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(54) Title: CRYSTAL STRUCTURE OF BACE AND USES THEREOF

(57) Abstract: This invention is directed to the three dimensional crystal structure of Beta-site APP Cleaving Enzyme (BACE), and to the use of this structure in rational drug design methods to identify agents that may interact with active sites of BACE. Such agents may represent new therapeutics in the treatment and/or prevention of Alzheimer's Disease.



#### CRYSTAL STRUCTURE OF BACE AND USES THEREOF

#### Field of the Invention

[ 0001] The present invention relates to the three dimensional crystal structure of Beta-site APP Cleaving Enzyme (BACE), and to the use of this structure in rational drug design methods to identify agents that may interact with active sites of BACE. Such agents may represent new therapeutics in the treatment and/or prevention of Alzheimer's Disease.

#### Background of the Invention

[ 0002] A characteristic pathology of Alzheimer's Disease is the build up of insoluble amyloid plaques in the brain. These proteinaceous plaques are composed of a 4KDa, 42 amino acid fragment of  $\beta$ -Amyloid Precursor Protein (APP) and is termed Amyloid  $\beta$ -peptide (A $\beta$ ). The mechanism of A $\beta$  production is hence of critical importance in understanding the onset and progress of Alzheimer's Disease. It has been shown that  $A\beta$  is derived from the proteolytic cleavage of a larger protein,  $\beta$ -amyloid precursor protein (APP). Two enzymes are responsible for this cleavage; first, the enzyme  $\beta$ -secretase cleaves APP at residue 671 (770aa isoform of APP numbering) and then γ-secretase cleaves at residue 716. More recently, the novel transmembrane aspartic protease BACE has been identified as being  $\beta$ -secretase. This protein is now a significant target in a therapeutic approach to Alzheimer's Disease. In rare cases of Alzheimer's Disease that are hereditary (Familial Alzheimer's Disease (FAD)) the disease phenotype has been isolated to mutations in the  $\beta$ -Amyloid Precursor Protein. One particular cohort, the 'Swedish mutation', exhibits a double mutation at the  $\beta$ -secretase cleavage site.

[ 0003] Based upon the role of BACE in Alzheimer's Disease, the elucidation of the three-dimensional structure of BACE, as well as its site of binding with APP, would have important implications in the treatment and/or prevention of Alzheimer's Disease and similar diseases associated with the

presence of insoluble amyloid plaques composed the 42 amino acid fragment of APP in the brain.

#### Summary of the Invention

[ 0004] The present invention provides a crystal of BACE complexed with an APP inhibitor peptide, as well as the three dimensional structure of BACE as derived by x-ray diffraction data of the BACE/APP inhibitor peptide crystal. Specifically, the three dimensional structure of BACE is defined by the structural coordinates shown in Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. The structural coordinates of BACE are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of various active sites of BACE, and the BACE/APP inhibitor peptide complex, including the APP binding site. The active site structures may then be used to design various agents which interact with BACE, as well as BACE complexed with an APP protein or peptide, or related molecules.

[ 0005] The present invention is also directed to an active site of an APP binding protein or peptide, and preferably the APP peptide binding site of BACE that is elucidated and derived from the three dimensional structure of BACE as defined by the relative structural coordinates set forth in Figure 1,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

In one embodiment of the present invention, the active site of the APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

[ 0007] In another embodiment, the active site of the APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the

relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

[ 0008] The present invention further provides a method for identifying an agent that interacts with an active site of BACE. The method comprises the steps of: (a) determining a putative active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å; and (b) performing various computer fitting analyses to identify an agent which interacts with the putative active site.

Interest invention also provides method for identifying an agent that interacts with an active site of an APP binding protein or peptide, preferably BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and (b) designing an agent using the three dimensional model generated in step (a).

The present invention also provides another method for [ 0010] identifying an agent that interacts with an active site of an APP binding protein or peptide, preferably BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and (b) designing an agent using the three dimensional model generated in step (a).

[ 0011] Finally, the present invention provides agents, and preferably inhibitors, identified using the foregoing methods. Small molecules or other agents which inhibit or otherwise interfere with the ability of BACE to cleave APP may be useful in the treatment and/or prevention of Alzheimer's Disease.

[ **0012**] Additional objects of the present invention will be apparent from the description which follows.

#### Brief Description of the Figure

[ 0013] Figure 1 provides the atomic structural coordinates for BACE and the APP inhibitor peptide as derived by X-ray diffraction of a crystal of the BACE and APP inhibitor peptide complex. "Atom type" refers to the atom whose coordinates are being measured. "Residue" refers to the type of residue of which each measured atom is a part - i.e., amino acid, cofactor, ligand or solvent. The

"x, y and z" coordinates indicate the Cartesian coordinates of each measured atom's location in the unit cell (Å). "Occ" indicates the occupancy factor. "B" indicates the "B-value", which is a measure of how mobile the atom is in the atomic structure ( $Å^2$ ).

#### Detailed Description of the Invention

[ 0014] As used herein, the following terms and phrases shall have the meanings set forth below:

Unless otherwise noted, "BACE" is Beta-site APP Cleaving Enzyme, [ 0015] and is the  $\beta$ -secretase enzyme that cleaves  $\beta$ -amyloid precursor protein (APP) at residue 671 (770aa isoform of APP numbering). After cleavage of APP by BACE, the remaining APP is cleaved at residue 716 by y-secretase, leaving a 42 amino acid fragment of APP that is found in the proteinaceous plaques of Alzheimer's patients. The amino acid sequence of BACE preferably has the amino acid sequence deposited with Swiss Prot under accession number P56817, including conservative substitutions. As used herein, BACE also includes "BACE peptides," which are molecules having less than the complete amino acid sequence of BACE. Preferably, BACE peptides include the active site in which BACE binds to and cleaves APP. Most preferably, the BACE peptide corresponds to amino acid residues 58-447 set forth in Figure 1 ("BACE<sub>58,447</sub>"), including conservative substitutions.

"APP" is  $\beta$ -amyloid precursor protein having the amino acid [ 0016] sequence deposited with Swiss Prot under accession number CAA31830, including conservative substitutions. As used herein, APP also includes "APP peptides," which are molecules having less than the complete amino acid sequence of APP. Preferably, APP peptides include the active site in which APP is cleaved by BACE.

An "APP inhibitor peptide" is a peptide which inhibits binding . [0017]between BACE and APP. Preferably, the APP peptide has the amino acid sequence SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE, where Sta is rare amino acid (S)-Statine.

An "APP binding protein or peptide" is a protein or peptide that [ 0018] binds APP and has a APP binding site, and includes but is not limited to BACE and BACE peptides.

Unless otherwise indicated, "protein" shall include a protein, [ 0019] protein domain, polypeptide or peptide.

"Structural coordinates" are the Cartesian coordinates [ 0020] corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using x-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original set provided in Figure 1 by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Figure 1.

An "agent" shall include a protein, polypeptide, peptide, nucleic [ 0021] acid, including DNA or RNA, molecule, compound or drug.

"Root mean square deviation" is the square root of the arithmetic [ 0022] mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates of BACE described herein. The present invention includes all embodiments comprising conservative substitutions of the noted amino acid residues resulting in same structural coordinates within the stated root mean square deviation.

The numbering of the amino acid residues identified in Figure  $oldsymbol{1}$ [ 0023] are based on the numbering of the full length BACE protein from the start of the signal sequence. It will be obvious to the skilled practitioner that the numbering of the amino acid residues of BACE may be different than that set forth herein or may contain certain conservative amino acid substitutions that yield the same

three dimensional structures as those defined in Figure 1. Corresponding amino acids and conservative substitutions in other isoforms or analogues are easily identified by visual inspection of the relevant amino acid sequences or by using commercially available homology software programs (e.g., MODELLAR, MSI, San Diego, CA).

[ 0024] "Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic) and includes substitutions having an inconsequential effect on the three dimensional structure of BACE, with respect to the use of this structure for the identification and design of agents which interact with BACE, for molecular replacement analyses and/or for homology modeling.

[ 0025] As used herein, an "active site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug) via various covalent and/or non-covalent binding forces. Preferably, the active site of BACE corresponds to the site in which BACE cleaves the APP molecule.

I 0026] As such, the active site of BACE may include, for example, both the actual site in which BACE binds and cleaves APP, as well as accessory binding sites adjacent or proximal to the actual binding site that nonetheless may affect the ability of BACE to bind and cleave APP, either by direct interference with the actual site of binding or by indirectly affecting the steric conformation or charge potential of the BACE molecule and thereby preventing or reducing the ability of BACE to bind to APP at the actual binding site. As used herein, an active site also includes BACE or BACE analog residues which exhibit observable NMR perturbations in the presence of a binding ligand, such as APP or an APP peptide. While such residues exhibiting observable NMR perturbations may not necessarily be in direct contact with or immediately

proximate to ligand binding residues, they may be critical to BACE residues for rational drug design protocols.

[ 0027] The present invention is directed to a crystallized complex of BACE and an APP inhibitor peptide that effectively diffracts X-rays for the determination of the structural coordinates of the complex. As used herein, BACE preferably corresponds to BACE<sub>58-447</sub> as set forth in Figure 1, with the N-terminal domain consisting of amino acid residues 58-207 shown in Figure 1, and the C-terminal domain consisting of amino acid residues 208-447 shown in Figure 1. The APP inhibitor peptide is preferably SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE.

[ 0028] Using the crystal complex of the present invention, X-ray diffraction data can be collected by a variety of means in order to obtain the atomic coordinates of the crystallized molecule or molecular complex. With the aid of specifically designed computer software, such crystallographic data can be used to generate a three dimensional structure of the molecule or molecular complex. Various methods used to generate and refine the three dimensional structure of a crystallized molecule or molecular structure are well known to those skilled in the art, and include, without limitation, multiwavelength anomalous dispersion (MAD), multiple isomorphous replacement, reciprocal space solvent flattening, molecular replacement, and single isomorphous replacement with anomalous scattering (SIRAS).

[ 0029] Accordingly, the present invention also provides the three dimensional structure of BACE as derived by x-ray diffraction data of the BACE/APP inhibitor peptide crystal. Specifically, the three dimensional structure of BACE is defined by the structural coordinates shown in Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å, preferably not more than 1.0Å, and most preferably not more than 0.5Å. The structural coordinates of BACE are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of various active sites of BACE, and the BACE/APP inhibitor peptide complex, including the APP or APP peptide binding site. The active site

structures may then be used to design agents with interact with BACE, as well as BACE complexed with APP, an APP peptide or related molecules.

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[ 0030] The present invention is also directed to an active site of an APP binding protein or peptide, preferably the APP peptide binding site of BACE, which comprises the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

In another preferred embodiment, the active site of an APP [ 0031] binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

[ 0032] Another aspect of the present invention is directed to a method for identifying an agent that interacts with an active site of BACE comprising the steps of: (a) determining an active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than

1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å; and (b) performing computer fitting analysis to identify an agent which interacts with said active site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the putative active site and the identified agent, by (a) generating a three dimensional model of the putative active site of a molecule or molecular complex using homology modeling or the atomic structural coordinates of the active site, and (b) determining the degree of association between the putative active site and the identified agent. Three dimensional models of the putative active site may be generated using any one of a number of methods known in the art, and include, but are not limited to, homology modeling as well as computer analysis of raw data generated using crystallographic or spectroscopy data. Computer programs used to generate such three dimensional models and/or perform the necessary fitting analyses include, but are not limited to: GRID (Oxford University, Oxford, UK), MCSS (Molecular Simulations, San Diego, CA), AUTODOCK (Scripps Research Institute, La Jolla, CA), DOCK (University of California, San Francisco, CA), Flo99 (Thistlesoft, Morris Township, NJ), Ludi (Molecular Simulations, San Diego, CA), QUANTA (Molecular Simulations, San Diego, CA), Insight (Molecular Simulations, San Diego, CA), SYBYL (TRIPOS, Inc., St. Louis. MO) and LEAPFROG (TRIPOS, Inc., St. Louis, MO).

Interpresent invention also provides a method for identifying an agent that interacts with an active site of an APP binding protein or peptide, and preferably the APP peptide binding site on BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å;

and (b) designing an agent using the three dimensional model generated in step (a). In another preferred embodiment, the active site of the APP binding protein or peptide is generated using the three dimensional model defined by the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

The effect of such an agent identified by computer fitting analyses [ 0034] on the APP binding protein or peptide may be further evaluated by obtaining or synthesizing the agent, and contacting the identified agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide. Preferably, the APP binding protein or peptide is BACE (or a BACE peptide), and the agent is a potential inhibitor of binding between BACE (or a BACE peptide) and APP (or an APP peptide). Therefore, in the preferred embodiment, the agent is contacted with BACE (or a BACE peptide) in the presence of APP (or a APP peptide), to determine the ability of the agent to inhibit binding between BACE (or the BACE peptide) and APP (or the APP peptide). Depending upon the action of the agent on the active site, the agent may act either as an inhibitor or activator of the BACE/APP binding. Assays may be performed and the results analyzed to determine whether the agent is an inhibitor (i.e., the agent may reduce or prevent binding affinity between BACE and APP), an activator (i.e., the agent may increase binding

affinity between BACE and APP), or has no effect on the interaction between BACE and APP. Agents identified using the foregoing methods, and preferably inhibitors of BACE cleavage of APP, may then be tested as therapeutics in the treatment and/or prevention of Alzheimer's Disease, and other diseases that are also characterized by the presence of the 42 amino acid fragment of APP in the proteinaceous plaques of the brain.

[ 0035] Various molecular analysis and rational drug design techniques are further disclosed in U.S. Patent Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published WO 99/09148, the contents of which are hereby incorporated by reference.

[ 0036] Finally, the present invention is also directed to the agents, and preferably the inhibitors, identified using the foregoing methods. Such agents may be a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, or drug, and preferably are small molecules that effectively inhibit binding between BACE and APP or an APP peptide. Such molecules may be useful in treating, preventing or inhibiting progression of Alzheimer's Disease.

[ 0037] The present invention may be better understood by reference to the following non-limiting Example. The following Example is presented in order to more fully illustrate the preferred embodiments of the invention, and should in no way be construed as limiting the scope of the present invention.

#### Example 1

#### A. Methods

[ 0038] Cloning of Human BACE1. Human polyA+ mRNA from whole brain (Clontech) was converted to cDNA by random-priming using Thermoscript RT-PCR System, according to the manufacturer's protocol (Lifetechnologies). This cDNA was amplified by PCR using the forward and reverse primers, 5' GCTCTAGAACCCAGC ACGGCATCCGGCTG 3' (XbaI site indicated by underlined sequence; nts. 517-537 in accession no. AF190725) and 5' CCAAGCATGCGGCCGCAATAGGCTATGGTCA TGAGGGTTGAC 3' (NotI site

indicated by underlined sequence; nts. 1809-1833; bold "A" indicates additional nucleotide to permit in-frame translation of the Fc chimera; see below), respectively. PCR was accomplished using Expand Long Polymerase kit according to the manufacturer's conditions (Roche Biochemicals; buffer #3), with PCR cycling consisting of an initial denaturing step at 95°C for 3min, 30-40 cycles of denaturation at 94°C for 30sec, annealing at 65°C for 30sec, elongation at 68°C for 1min 30sec, followed by a final elongation at 68°C for 5min. The PCR products were run on a 1% agarose gel. The appropriate band was cut out of the gel, purified by Quantum Prep Freeze 'N Squeeze DNA Extraction Columns (Bio-Rad), and cloned into the Spel/Notl sites of the mammalian expression vector, pED/Fc (Kaufman, RJ et al., 1991, Nucl. Acids. Res. 19:4485-4490).

[ 0039] An intermediate construct contained the honey bee meletin secretory leader fused to the the prodomain and coding region of BACE1, just upstream to the predicted transmembrane domain of BACE1 (Vassar, R. et al., 1999, Science 286:735-741). The absence of the predicted hydrophobic transmembrane domain in this construct would permit soluble secreted BACE.Fc protein to be extracted from the conditioned medium. Downstream of BACE1 was an engineered enterokinase cleavage site followed by sequence encoding the Fc portion of immunoglobulin IgG. The final construct contained the BACE1.Fc gene, flanked by Sall and EcoRI in pED/Fc, cloned into the Sall/EcoRI sites of the mammalian expression vector, pHTop, a derivative of pED, in which the majority of the adenovirus major late promoter was replaced by six repeats of a bacterial tetracycline operator (described in Gossen et al, 1992, PNAS, 89:5547-5551). Sequencing of the BACE1.Fc recombinant gene was accomplished by BigDye terminator dideoxy sequencing using an ABI3700. Sequence analyses was accomplished using DNAstar software package.

[ 0040] Expression of Human BACE1. The vector, pHTOP, with the BACE1.Fc insert, contains the dihydrofolate reductase gene and when introduced in the cell line CHO/A2 (see description below) functions very

efficiently and high expressers can be selected by isolating cells surviving in high methotrexate concentrations. The CHO/A2 cell line is derived from CHO DUKX B11 (Urlaub and Chasin, 1980, PNAS USA 77:4216-4220) by stably integrating a transcriptional activator (tTA), a fusion protein between the Tet repressor and the herpes virus VP16 transcriptional domain (Gossen et al). A CHO cell line expressing extracellular BACE1. Fc was established by transfecting (lipofection) pHTopBACE1. Fc into CHO/A2 cells and selecting clones in 0.02 and 0.05 µM methotrexate. The conditioned media from multiple clones were screened by Western blot using a (mouse) anti-human IgG. Fc HRP antibody. The same clones were also metabolically labeled with 35 S (met/cys). The best clone, determined by virtue of its high expression, was one which resulted from 0.05 µM MTX selection and was chosen to be scaled up for roller bottle conditioned media production (4 Liters). The conditioned media was then used for purification. The expressed protein has residues 22-460 and nine extra residues at the C-terminal (an artefact from cloning and remains of the EK cleavage site).

[ 0041] Purification of BACE1. For the purification of BACE the 102 liters of conditioned media was used. During purification the activity of the enzyme was estimated at room temperature by continuously monitoring the fluorescent intensity for 5-10 min. at 420 nm (ext – 320 nm) Abz-Ser-Glu-Val-Asn-Leu-Asp-Ala-Glu-Phe-Arg-Dpa (Abz = Amino benzoic acid, Dpa = 9,10-diphenylanthracene) as the substrate. The reaction mixture contained 20  $\mu$ M of substrate, different amounts of enzyme in 0.5 ml of 20 mM Tris-HCl pH 8.0 and 100 mM NaCl. The concentrated material of conditioned media(1.6 l) was applied to column (2.8 x 12 cm) containing ImmunoPure Immobilized Protein A agarose (Pierce, Il, USA) equilibrated in PBS buffer. The speed of application was 2 ml/min. The column was washed with 1 litre of PBS buffer and the BACE-Fc protein was eluted by ImmunoPure IgG Elution Buffer (Pierce, Il, USA). The fractions containing protein were immediately neutralized by 1 M Tris-HCl to pH 8.0.

crystallization experiments.

The obtained protein material was treated with Enterokinase at ſ 00421 25°C. The ratio of BACE-Fc to Enterokinase was 3000:1 and the time of reaction was 3 hrs. The reaction was stopped by removing Enterokinase from reaction mixture by applying the protein to a column (1 x 5 cm) containing soybean trypsin inhibitor agarose (Sigma, Mo, USA) equilibrated in 20 mM Tris-HCL pH 8.0 containing 100 mM NaCl (speed was 1 ml/min). The flow through material contained BACE and cleaved Fc. Cleaved Fc was removed from BACE by flowing through a protein A column equilibrated in 20 mM Tris-HCl pH 8.0. BACE was partially de-glycosylated using PNGase F (New England [ 0043] Labs., Ma, USA). 8-9 µg of PNGase was added to 1 mg of BACE and the incubation was carried at 37° C for 16 hrs. The additional 5-6 µg of PNGase was added to each mg of BACE and incubation was continued for another 4 hrs. The purified BACE was separated from PNGase by HPLC size-exclusion chromatography using 21.5 x 30 cm G-3000SW column (TosoHaas, Pa, USA) equilibrated in 20 mM tris-HCL pH 8.0 containing 200 mM NaCl. (Speed of elution was 3 ml/min). The purified BACE was concentrated and used for

[ 0044] N-terminal sequencing of purified BACE reveals a mixture of protein species, with the major sample having the processing domain cleaved and beginning at residue 47 (all numbering refers to full length BACE; accession code: A59090) and a minor sample which had not been cleaved beginning at residue 22. A smaller sample with sequence MTIAY was also detected.

Crystallization. The crystals were grown using the hanging drop vapour diffusion method. The protein was concentrated to mg/ml in 20mM Tris pH 7.5, 200mM sodium chloride. Inhibitor peptide sequence is SEVNStaVAEF, where Sta is the rare amino acid (S)-Statine. It was concentrated to 100mM in 100% DMSO and mixed with concentrated protein in a two-fold peptide excess to form the complex. 1  $\mu$ l of complex was added to 1  $\mu$ l of well solution containing 100mM Sodium Cacodylate pH6.5, 25% PEG8K, 300mM lithium sulphate. Plate-like crystal clusters grew within one week to dimensions of 200

 $\mu$ m x 400  $\mu$ m x 75  $\mu$ m. Single crystals were transferred to a stabilizing, cryoprotectant solution which contained the well solution plus 25% Glycerol for a brief, 10 second, soak and then frozen in liquid nitrogen. X-ray diffraction crystals had space group I222, and unit cell parameters a=86.627, b=130.861, c=130.729, and  $\alpha$ =  $\beta$ = $\gamma$ =90°.

#### B. Results

Expressed in CHO cells as a fc fusion protein and, after purification, cleavage and partial deglycosylation, complexed with peptide inhibitor and crystallized. Crystals diffracted to 2.3Å and the structure was solved using the technique of molecular replacement. The search model used was derived from cod atlantic Pepsin and contained 63% of the final number of atoms. The density modified maps obtained using a poly-alanine version of the search model (39% of the final atoms) provided sufficient information to build all but 12 amino acids. The final model contains residues from 59 to 448 (using full length numbering), all 9 residues of the statine inhibitor and 360 water molecules. Of the four predicted N-linked glycosylation sites only two have interpretable electron density.

[ 0047] The overall shape of the BACE protein is spherical and is composed of two distinct domains, an N-terminal (58-207) and a C-terminal (208-447). With the first thirteen amino acids (58-71) being packed against residues 238-243. There is a significant cleft-like channel across one surface of the interface between the domains. This contains the inhibitor peptide and conserved aspartic acid motifs that define the active sites of aspartic proteases.

[ 0048] The N-terminal domain is composed of a single a-helix preceding the loop joining the two domains and thirteen  $\beta$ -strands. The larger C-terminal domain has a total of seventeen  $\beta$ -strands and three  $\alpha$ -helices. The overall topology is characterised by an eight stranded antiparallel interdomain  $\beta$ -sheet. This central sheet comprises the majority of the active site residues including the two conserved aspartates (one from each domain:93 and 289). Asp93 and

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Asp289 define the position of a pseudo two-fold axis for the central  $\beta$ -sheet. Outside of this symmetry the two domains differ significantly. The N-terminal domain has an extra two strands extending the central sheet. In addition, there are two anti-parallel  $\beta$ -sheets above and below the central sheet composed of three and four  $\beta$ -strands respectively. Residues from the upper sheet (131-135) fold over the active site aspartates and form a 'flap' over the centre of the peptide binding cleft.

[ 0049] The C-terminal domain contains two lobes in addition to the strands which from the central  $\beta$ -sheet. These are weakly homologous to known aspartic protease structures. The binding pocket for the P1`and P3`positions are instead derived from three  $\beta$ -turns 388-391, 284-286 and 255-261.

[ 0050] There are a total of six cysteine residues in BACE. Each of these is involved in a disulphide interaction. The pattern of disulphide crosslinking, Cys278-Cys443, Cys380-Cys330, Cys420-Cys216 are unique in the aspartic proteases known to date.

[ 0051] A novel aspartic protease. The first attempts to study the relationship of function to structure of an Apartic proteases began in the 1930s with Pepsin. Since then this rich field of research has been successfully applied to the design of clinically used inhibitors in only one system; HIV protease. The reasons for this are related more to the validity of the pharmacological target than the efficacy of inhibitors.  $\beta$ -secretase has been described as a novel protease and has been shown to be linked to the onset and progression of Alzheimer's disease.

[ 0052] From a gross viewpoint the overall fold and domain organization is very similar to that of a canonical aspartic protease. The comparison at a more detailed level reveals a significant number of differences. The active site is characterized by two aspartic residues surrounded by a conserved set of hydrogen bonds termed a 'fireman's grip'. This is reproduced in the -secretase structure presented here. The characteristic flap which wraps over the active site in pepsin is absent from the C-terminal domain in a manner analogous to

cathepsin D. In  $\beta$ -secretase the critical main chain amide hydrogen bond to the carboxyl group of statine is maintained by Thr133 from this flap. The amide of the statine makes a hydrogen bond to the carboxyl group of Gly95, emphasizing that the statine residue occupies both the P1 and P1` position.

Enzyme Mechanism. It has been shown that  $\beta\mbox{-secretase}$  cleavage [ 0053] is dependent on proximity to the cell membrane. Both  $\beta\mbox{-secretase}$  and its substrate APP have putative transmembrane regions. Our expressed BACE construct finishes one amino acid before the predicted transmembrane region. The final residue in the current structure is Ile447, thirteen residues away from the beginning of the putative transmembrane domain. In the current crystal structure Ile447 is only 6Å away from the P3 Glutamic acid of the inhibitor suggesting a role for the remaining C-terminal residues in the enzyme mechanism. The Statine residue of the inhibitor peptide is bound at the S1 position within the active site. The position of the C-3 hydroxyl group, coplanar to and within hydrogen bonding distance of both aspartate 93 and 289 carboxyl groups, confirms that the rare amino acid mimics the tetrahedral transition state i.e the intermediate of peptide-bond hydrolysis. The distance between the oxygen atoms of Asp93 and Asp289 is 2.8Å, strongly suggesting a shared proton atom and a classic aspartic protease pK profile for these side-chains and a common enzyme mechanism to other known aspartic proteases.

Inhibitor binding. The inhibitor peptide binds in an extended form along a 20Å groove formed at the interface between the domains. The conserved catalytic aspartic residues lie at the middle of this groove. The bound peptide consists of 8 amino acids plus a statine amino acid at position 5. There is contiguous electron density for the whole peptide. The statine based inhibitor used in this study has been show to inhibit the  $\beta$ -secretase enzyme with nanomolar efficiency. The peptide sequence is based on the P10 to P4` APP751 Sweedish family mutation. This mutation of a Lys-Asn at the P2 position and Met-Leu at the P1 position is strongly correlated to the early onset of

Alzheimer's disease. The inhibitor peptide utilizes Statine's Leucyl like side-chain to explore this interaction. Due to the di-peptide nature of Satine the P1' position of the substrate is shifted to P2' leaving an empty S1' pocket. The  $\beta$ -secretase enzyme appears to have a novel preference for an apartate or glutamate at the P1' position whereas other aspartic proteases show a preference for hydrophobic residues. This unusual preference for a negatively charged P1' amino acid is explained by the guanadinium group of Arg189 forming part of the putative S1' pocket. Even at the acidic pH optima of BACE the arginine side chain would form a positively charged environment for the possibly protonated carboxyl side-chain atoms.

[ 0055] The S1 and S3 binding pockets are a contiguous, hydrophobic pocket formed by the side-chain of residues Tyr132, Phe169, Ile171, Trp176, Ile179 and main chain atoms of Gly74, and Gln73. This packing of inhibitor P1 and P3 side chains has been seen in previous aspartic protease complexes.

[ 0056] The canonical APP cleavage site for b-secretase appears to have a preference for a small hydrophobic residues at the P2` position. The side chain of the valine residue bound in the putative S2` site of  $\beta$ -secretase appears to not make any significant interactions with the protein, its main chain however forms a tight set of hydrogen bonds to the backbone carboxyl of Gly 95 and the sidechain OH of Tyr259. In turn, Tyr259 is held rigidly in place by an edge-pi interaction with Trp258, which packs against the guanadinium group of Arg256.

[ 0057] Swedish mutation. Autosomal dominant mutations identified on the  $\beta$ -amyloid precusor protein have been correlated to early-onset cases of Alzheimer's disease. These have been shown to cluster around the three canonical cleavage sites. A double (the so-called Swedish) mutation of Lys670-Met671 (770aa isoform of APP numbering) to Asn-Leu causes an increase in the overall quantity of A $\beta$  detectable in the plasma and in the medium of cultured fibroblasts from carriers of the Swedish mutation. These two amino acids lie at the P2 and P1 positions of the  $\beta$ -secretase active site. The statine based inhibitor used here is based on this Swedish mutation. A methionine at position

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P1 would clearly be accommodated but would loose the van Der Waal's complentarity exhibited by the statine side-chain to Leu90 and Ile178. The C6 atom of the methione would make supplement the hydrophobic interaction to Phe169.

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#### Table 1

Residues of BACE Within 4Å of Peptide Inhibitor SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296, ARG368

Residues of BACE Within 8Å of Peptide Inhibitor
LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94,
GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133,
GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171,
ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183,
TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191,
ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286,
ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294,
LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383,
ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391,
THR392, VAL393, GLY395, ALA396, ILE447

[ 0058] All publications mentioned herein above, whether to issued patents, pending applications, published articles, deposited sequences, or otherwise, are hereby incorporated by reference in their entirety. While the foregoing invention has been described in some detail for purposes of clarity and understanding, it will be appreciated by one skilled in the art from a reading of the disclosure that various changes in form and detail can be made without departing from the true scope of the invention in the appended claims.

What is claimed is:

- 1. A crystallized complex of Beta-site APP Cleaving Enzyme (BACE) and SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE.
- 2. The crystallized complex of Claim 1, wherein BACE has an N-terminal domain consisting of amino acid residues 58-207 shown in Figure 1, and a C-terminal domain consisting of amino acid residues 208-447 shown in Figure 1.
- 3. An active site of an APP binding protein or peptide comprising the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 4. The active site of Claim 3, wherein the  $\pm$  a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 5. The active site of Claim 3, wherein the  $\pm$  a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 6. An active site of an APP binding protein or peptide comprising the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171,

ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

- 7. The active site of Claim 6, wherein the  $\pm$  a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 8. The active site of Claim 6, wherein the  $\pm$  a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 9. A method for identifying an agent that interacts with an active site of Beta-site APP Cleaving Enzyme (BACE), comprising the steps of:
- (a) determining an active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) performing computer fitting analysis to identify an agent which interacts with said active site.
- 10. The method of Claim 9, wherein the  $\pm$  a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 11. The method of Claim 9, wherein the  $\pm$  a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.

- A method for identifying an agent that interacts with an 12. active site of an APP binding protein or peptide, comprising the steps of:
- generating a three dimensional model of an active site of (a) an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- designing an agent using the three dimensional model (b) generated in step (a).
- The method of Claim 12, wherein the  $\pm$  a root mean 13. square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- The method of Claim 12, wherein the  $\pm$  a root mean 14. square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- The method of Claim 12, wherein the agent is designed by 15. performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- The method of Claim 12, further comprising the steps of: 16. (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.

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12. A method for identifying an agent that interacts with an active site of an APP binding protein or peptide, comprising the steps of:

- generating a three dimensional model of an active site of (a) an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- designing an agent using the three dimensional model (b) generated in step (a).
- The method of Claim 12, wherein the  $\pm$  a root mean 13. square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- The method of Claim 12, wherein the  $\pm$  a root mean 14. square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- The method of Claim 12, wherein the agent is designed by 15. performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- 16. The method of Claim 12, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.

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- 17. The method of Claim 12, wherein the APP binding protein or peptide is BACE.
- 18. The method of Claim 17, wherein the agent is a potential inhibitor of binding between BACE and APP.
- 19. The method of Claim 18, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with BACE in the presence of APP.
- 20. A method for identifying an agent that interacts with an active site of an APP binding protein or peptide, comprising the steps of:
- (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) designing an agent using the three dimensional model generated in step (a).
- 21. The method of Claim 18, wherein the  $\pm$  a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.

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- 22. The method of Claim 20, wherein the  $\pm$  a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 23. The method of Claim 20, wherein the agent is designed by performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- 24. The method of Claim 20, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.
- 25. The method of Claim 20, wherein the APP binding protein or peptide is BACE.
- 26. The method of Claim 25, wherein the agent is a potential inhibitor of binding between BACE and APP.
- 27. The method of Claim 26, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with BACE in the presence of APP.
  - 28. An agent identified by the method of Claim 9.
  - 29. An agent identified by the method of Claim 12.
  - 30. An agent identified by the method of Claim 20.

Figure 1

		Ato	m Res	5.		X	<u>Y</u> .	Z		
. = 4		Typ		_				<del>_</del>	1 00	E0 33
MOTA	1				58	31.563	49.775	16.324		59.33
MOTA	2	CA	GLY		58	32.861	50.358	16.764		58.44
ATOM	3	C	GLY		58	33.594	49.446	17.727		57.81
MOTA	4	0	GLY		58	34.067	48.331	17.333		56.66
ATOM	5	N	SER		59	33.712	49.888	18.975		56.66
ATOM	6	CA	SER		59	34.391	49.094	20.015		55.45
ATOM	7	C	SER		59	33.560	49.088	21.293		53.77
ATOM	8	0	SER		59	32.978	50.147	21.704 20.309		54.40
ATOM	9	CB	SER		59	35.781	49.668			55.79
ATOM	10	OG	SER		59		50.952 47.924	20.899 21.927		57.07 49.96
ATOM	11	И	PHE		60	33.480 32.719	47.772	23.181		45.72
ATOM	12	CA	PHE		60 60	33.681	47.269	24.247		44.79
MOTA MOTA	13 14	C 0	PHE	A	60	33.495	46.160	24.831		45.45
ATOM	15	CB	PHE		60	31.564	46.790	22.976		43.28
ATOM	16	CG	PHE		60	30.557	47.249	21.957		41.00
ATOM	17		PHE		60	30.875	47.267	20.602		40.54
ATOM	18		PHE		60	29.301	47.701	22.355		40.58
ATOM	19	CE1			60	29.954	47.731	19.658		39.88
ATOM	20	CE2	PHE		60	28.375	48.166	21.419		39.50
ATOM	21	CZ	PHE		60	28.704	48.182	20.070		39.23
ATOM	22	N	VAL		61	34.709	48.073	24.500	1.00	43.29
ATOM	23	CA	VAL		61	35.763	47.756	25.483	1.00	43.19
ATOM	24	C	VAL		61	35.243	47.069	26.738	1.00	41.81
ATOM	25	0	VAL		61	35.876	46.099	27.247	1.00	42.54
MOTA	26	CB	VAL	A	61	36.532	49.035	25.895	1.00	43.62
MOTA	27	CG1	VAL	Α	61	37.069	49.730	24.655	1.00	44.38
ATOM	28	CG2	VAL	A	61	35.621	49.975	26.676	1.00	44.28
ATOM	29	N	GLU	Α	62	34.114	47.542	27.252		40.86
ATOM	30	CA	GLU	A	· 62	33.517	46.959	28.470		40.02
ATOM	31	C	GLU	A	62	33.208	45.473	28.320		36.45
MOTA	32	0	GLU		62	33.366	44.685	29.301		36.49
MOTA	33	CB	GLU		62	32.226	47.700	28.832		43.76
MOTA	34	CG	GLU		62	32.399	48.895	29.764		48.74
ATOM	35	CD	GLU		62	32.743	48.486	31.188		51.91
ATOM	36	OE1			62	32.317	47.387	31.612		53.41
ATOM	37	OE2	GLU		62	33.423	49.271	31.890 27.129		53.64 30.86
MOTA	38	N	MET		63	32.780	45.062 43.643			27.79
ATOM	39	CA	MET MET		63 63	32.421 33.491	42.741	26.896 26.279		26.02
MOTA	40	C	MET		63	33.354	41.476	26.310		25.25
ATOM	41 42	O CB	MET		63		43.578	26.078		25.63
MOTA MOTA	43	CG	MET		63	29.942	44.133	26.858		24.89
ATOM	44	SD	MET		63	28.392	44.180	25.960		23.85
ATOM	45	CE	MET		63	28.431	45.848	25.316		24.18
ATOM	46	N	VAL		64	34.551	43.330	25.736		23.39
MOTA	47	CA	VAL		64	35.639	42.516	25.143		20.76
ATOM	48	C	VAL		64	36.263	41.634	26.216		20.06
ATOM	49	ō	VAL		64	36.531	42.095	27.370		18.87
MOTA	50	СВ	VAL		64	36.740	43.407	24.517		21.16
ATOM	51		VAL		64	37.958	42.567	24.151		18.99
ATOM	52		VAL		64	36.193	44.092	23.266		21.01
MOTA	53	N	ASP		65	36.487	40.373	25.869		18.21
ATOM	54	CA	ASP		65	37.091	39.397	26.800		18.56
ATOM	55	C	ASP		65	36.280	39.174	28.071		17.80
ATOM	56	0	ASP		65	36.869	38.964	29.165		16.29
ATOM	57	CB	ASP	Α	65	38.508	39.829	27.194		21.53
MOTA	58	CG	ASP		<sup>.</sup> 65	39.409	40.055	25.993	1.00	22.65

				_		20 162	20 454	04 030	1 00 22 75
MOTA	59	OD1	ASP	A	65	39.162	39.451	24.930	1.00 23.75
MOTA	60	OD2	ASP	Α	65	40.375	40.831	26.117	1.00 24.72
ATOM	61	N	ASN	Α	66	34.955	39.209	27.969	1.00 16.59
MOTA	62	CA	ASN		66	34.090	38.987	29.156	1.00 16.58
						33.719	37.508	29.274	1.00 17.20
ATOM	63	C	ASN		66				1.00 19.23
MOTA	64	0	ASN	A	66	32.815	37.125	30.070	
MOTA	65	CB	ASN	Α	66	32.817	39.845	29.059	1.00 14.62
ATOM	66	CG	ASN	Α	66	31.967	39.516	27.835	1.00 15.57
ATOM	67		ASN		66	32.381	38.714	26.937	1.00 16.31
						30.788	40.120	27.760	1.00 14.85
ATOM	68		ASN		66				1.00 17.73
MOTA	69	N	LEU		67	34.409	36.664	28.515	
MOTA	70	CA	LEU	Α	67	34.134	35.206	28.529	1.00 17.36
ATOM	71	С	LEU	A	67	35.295	34.328	28.985	1.00 16.04
MOTA	72	0	LEU	A	67	36.499	34.701	28.842	1.00 16.38
MOTA	73	CB	LEU		67	33.707	34.757	27.128	1.00 17.19
					67	32.226	34.504	26.839	1.00 18.63
MOTA	74	CG	LEU						1.00 16.94
ATOM	75		LEU		67	31.349	35.604	27.407	
ATOM	76	CD2	LEU	A	67	32.049	34.375	25.330	1.00 18.67
ATOM	77	N	ARG	Α	68	34.956	33.166	29.531	1.00 14.58
ATOM	78	CA	ARG	Α	68	35.961	32.173	29.973	1.00 16.73
ATOM	79	C	ARG		68	35.394	30.775	29.717	1.00 15.78
	80		ARG		68	34.154	30.610	29.500	1.00 13.85
MOTA		0					32.349	31.459	1.00 18.19
MOTA	81	CB	ARG		68	36.299			
MOTA	82	CG	ARG	Α	68	37.086	33.623	31.766	1.00 21.67
MOTA	83	CD	ARG	Α	68	37.571	33.646	33.213	1.00 23.25
ATOM	84	NE	ARG	A	68	36.462	33.653	34.165	1.00 26.34
MOTA	85	CZ	ARG	Α	68	36.598	33.500	35.482	1.00 27.29
ATOM	86	-	ARG		68	37.802	33.324	36.015	1.00 25.91
	87	NH2			68	35.530	33.527	36.271	1.00 26.77
MOTA						36262	29.769	29.726	1.00 14.89
MOTA	88	N	GLY		69				
MOTA	89	CA	GLY		69	35.816	28.409	29.486	1.00 15.62
MOTA	90	С	GLY	Α	69	36.505	27.806	28.277	1.00 16.66
MOTA	91	0	GLY	Α	69	37.526	28.367	27.771	1.00 15.60
ATOM	92	N	LYS	A	70	35.989	26.676	27.804	1.00 17.25
ATOM	93	CA	LYS		70	36.556	25.973	26.629	1.00 16.95
ATOM	94	C		A	70	35.472	25.138	25.949	1.00 16.87
			LYS		70	34.394·	24.864	26.562	1.00 17.19
MOTA	95	0						27.058	1.00 18.62
MOTA	96	CB	LYS		70	37.737	25.092		
MOTA	97	CG		A	70	37.518	24.303	28.348	1.00 19.97
ATOM	98	CD	LYS	Α	70	38.737	23.446	28.667	1.00 22.43
ATOM	99	CE	LYS	Α	70	38.538	22.611	29.926	1.00 23.77
ATOM	100	NZ	LYS		70	39.660	21.638	30.129	1.00 22.43
ATOM	101	N	SER		71	35.714	24.729	24.706	1.00 15.11
	102	CA	SER		71	34.706	23.950	23.940	1.00 14.34
ATOM							22.730	24.667	1.00 14.36
ATOM	103	C	SER		71	34.155			
MOTA	104	0	SER	Δ	71		22 116	24 600	1 00 17 01
MOTA						32.918	22.446	24.600	1.00 13.81
MOTA	105	CB	SER		71	35.281	23.523	22.581	1.00 14.97
MOTA	105 106			A			23.523 22.743	22.581 22.732	1.00 14.97 1.00 15.41
		СВ	SER	A A	71	35.281	23.523	22.581	1.00 14.97
ATOM	106 107	CB OG N	SER SER GLY	A A A	71 71 72	35.281 36.456 35.024	23.523 22.743	22.581 22.732 25.362	1.00 14.97 1.00 15.41
ATOM	106 107 108	CB OG N CA	SER SER GLY GLY	A A A	71 71 72 72	35.281 36.456 35.024 34.588	23.523 22.743 22.005 20.815	22.581 22.732 25.362 26.072	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63
ATOM	106 107 108 109	CB OG N CA C	SER SER GLY GLY GLY	A A A A	71 71 72 72 72	35.281 36.456 35.024 34.588 33.661	23.523 22.743 22.005 20.815 21.022	22.581 22.732 25.362 26.072 27.262	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49
MOTA MOTA	106 107 108 109 110	CB OG N CA C	SER SER GLY GLY GLY GLY	A A A A	71 71 72 72 72 72	35.281 36.456 35.024 34.588 33.661 32.772	23.523 22.743 22.005 20.815 21.022 20.159	22.581 22.732 25.362 26.072 27.262 27.537	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.20
MOTA MOTA MOTA	106 107 108 109 110	CB OG N CA C O	SER SER GLY GLY GLY GLY	A A A A A	71 71 72 72 72 72 72 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814	23.523 22.743 22.005 20.815 21.022 20.159 22.129	22.581 22.732 25.362 26.072 27.262 27.537 27.979	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.20 1.00 16.78
MOTA MOTA	106 107 108 109 110 111	CB OG N CA C O N	SER GLY GLY GLY GLN GLN	A A A A A	71 71 72 72 72 72 72 73 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814 32.965	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.20 1.00 16.78 1.00 18.67
MOTA MOTA MOTA	106 107 108 109 110	CB OG N CA C O	SER SER GLY GLY GLY GLY	A A A A A	71 71 72 72 72 72 72 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369 23.570	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167 29.038	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.20 1.00 16.78 1.00 18.67
MOTA MOTA MOTA MOTA MOTA	106 107 108 109 110 111	CB OG N CA C O N	SER GLY GLY GLY GLN GLN	A A A A A A	71 71 72 72 72 72 72 73 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814 32.965	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369 23.570 23.858	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.20 1.00 16.78 1.00 18.67
ATOM ATOM ATOM ATOM ATOM ATOM	106 107 108 109 110 111 112 113 114	CB OG N CA C O N CA C	SER SER GLY GLY GLY GLN GLN GLN GLN	A A A A A A	71 71 72 72 72 72 73 73 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814 32.965 32.040 31.223	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369 23.570 23.858	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167 29.038	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.20 1.00 16.78 1.00 18.67
ATOM ATOM ATOM ATOM ATOM ATOM	106 107 108 109 110 111 112 113 114 115	CB OG N CA C O N CA C C O CB	SER SER GLY GLY GLY GLN GLN GLN GLN	A A A A A A A A	71 71 72 72 72 72 73 73 73 73 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814 32.965 32.040 31.223 33.852	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369 23.570 23.858 22.522	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167 29.038 29.967 30.401	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.78 1.00 18.67 1.00 18.70 1.00 19.81 1.00 20.09
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	106 107 108 109 110 111 112 113 114 115 116	CB OG N CA C O N CA C C C C C C C	SER SER GLY GLY GLY GLN GLN GLN GLN GLN	A A A A A A A A A	71 71 72 72 72 72 73 73 73 73 73 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814 32.965 32.040 31.223 33.852 34.924	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369 23.570 23.858 22.522 21.433	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167 29.038 29.967 30.401 30.493	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.78 1.00 18.67 1.00 18.70 1.00 19.81 1.00 20.09 1.00 24.21
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	106 107 108 109 110 111 112 113 114 115 116	CB OG N CA C O CA C C C C C C C C C C C C C C C	SER SER GLY GLY GLY GLN GLN GLN GLN GLN GLN	A A A A A A A A A A A A	71 71 72 72 72 72 73 73 73 73 73 73 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814 32.965 32.040 31.223 33.852 34.924 35.624	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369 23.570 23.858 22.522 21.433 21.400	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167 29.038 29.967 30.401 30.493 31.837	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.78 1.00 18.67 1.00 18.70 1.00 19.81 1.00 20.09 1.00 24.21 1.00 24.83
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	106 107 108 109 110 111 112 113 114 115 116 117	CB OG N CA C O CB CC CCB CCC CD OE1	SER SER GLY GLY GLY GLN GLN GLN GLN GLN GLN GLN GLN	A A A A A A A A A A A A A A A A A A A	71 71 72 72 72 72 73 73 73 73 73 73 73 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814 32.965 32.040 31.223 33.852 34.924 35.624 36.048	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369 23.570 23.858 22.522 21.433 21.400 22.467	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167 29.038 29.967 30.401 30.493 31.837 32.380	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.78 1.00 18.67 1.00 18.70 1.00 19.81 1.00 20.09 1.00 24.21 1.00 24.83 1.00 26.53
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	106 107 108 109 110 111 112 113 114 115 116	CB OG N CA C O N CA C C C C C C C C C	SER SER GLY GLY GLY GLN GLN GLN GLN GLN GLN GLN GLN	A A A A A A A A A A A A A A A	71 71 72 72 72 72 73 73 73 73 73 73 73	35.281 36.456 35.024 34.588 33.661 32.772 33.814 32.965 32.040 31.223 33.852 34.924 35.624	23.523 22.743 22.005 20.815 21.022 20.159 22.129 22.369 23.570 23.858 22.522 21.433 21.400	22.581 22.732 25.362 26.072 27.262 27.537 27.979 29.167 29.038 29.967 30.401 30.493 31.837	1.00 14.97 1.00 15.41 1.00 14.38 1.00 14.63 1.00 16.49 1.00 16.78 1.00 18.67 1.00 18.70 1.00 19.81 1.00 20.09 1.00 24.21 1.00 24.83

MOTA	121	CA	GLY	Α	74	31.292	25.429	27.688	1.00 15.83
MOTA	122	С	GLY	Α	74	31.939	26.746	28.068	1.00 15.56
MOTA	123	ō	GLY		74	32.837	26.799	28.962	1.00 17.53
			_					27.403	1.00 13.96
MOTA	124	N	TYR		75	31.517	27.814		
ATOM	125	CA	TYR		75	32.041	29.164	27.686	1.00 16.12
ATOM	126	С	TYR	Α	75	30.991	29.903	28.502	1.00 14.92
MOTA	127	0	TYR	Α	75	29.758	29.793	28.217	1.00 14.71
MOTA	128	СВ	TYR	Α	75	32.324	29.918	26.385	1.00 17.79
MOTA	129	CG	TYR		75	33.490	29.354	25.605	1.00 18.92
	130	CD1			75 75	33.326	28.271	24.742	1.00 19.83
MOTA									
MOTA	131	CD2			75	34.763	29.909	25.735	1.00 20.43
MOTA		· CE1			75	34.409	27.757	24.020	1.00 21.98
MOTA	133	CE2	TYR	Α	75	35.847	29.407	25.025	1.00 21.04
MOTA	134	CZ	TYR	Α	75	35.666	28.339	24.170	1.00 22.04
ATOM	135	OH	TYR	Α	75	36.746	27.882	23.456	1.00 22.86
ATOM	136	N	TYR	Α	76	31.432	30.653	29.507	1.00 13.66
ATOM	137	CA	TYR		76	30.478	31.360	30.368	1.00 12.95
					76	30.753	32.837	30.593	1.00 13.47
ATOM	138	C	TYR						
ATOM	139	0	TYR		76	31.901	33.345	30.391	1.00 13.77
ATOM	140	ĊВ	TYR		76	30.395	30.662	31.725	1.00 13.31
ATOM	141	CG	TYR	A	76	31.723	30.548	32.446	1.00 14.55
MOTA	142	CD1	TYR	A	76	32.601	29.497	32.174	1.00 16.16
ATOM	143	CD2	TYR	A	76	32.105	31.495	33.392	1.00 15.68
ATOM	144	CE1			76	33.829	29.392	32.832	1.00 17.64
ATOM	145	CE2	TYR		76	33.329	31.402	34.055	1.00 18.14
					76	34.183	30.348	33.770	1.00 18.24
MOTA	146	CZ	TYR						
ATOM	147	OH	TYR		76	35.390	30.252	34.428	1.00 21.79
ATOM	148	N	VAL		77	29.716	33.546	31.017	1.00 12.55
ATOM	149	CA	VAL	A	77	29.844	34.980	31.298	1.00 14.17
MOTA	150	С	VAL	Α	77	29.390	35.225	32.727	1.00 15.16
ATOM	151	0	VAL	Α	77	28.564	34.439	33.283	1.00 16.09
ATOM	152	СВ	VAL	Δ	77	28.975	35.821	30.336	1.00 13.43
ATOM	153		VAL		77	27.495	35.528	30.567	1.00 11.59
	154		VAL		77	29.281	37.305	30.524	1.00 10.74
ATOM									
ATOM	155	N	GLU		78	29.905	36.276	33.352	1.00 16.88
MOTA	156	CA	GLU		78	29.486	36.571	34.731	1.00 17.45
MOTA	157	С	GLU		78	28.178	37.345	34.706	1.00 16.89
ATOM	158	0	GLÜ	Α	78	27.961	38.239	33.826	1.00 14.65
ATOM	159	ÇВ	GLU	A	78	30.538	37.392	35.479	1.00 19.11
ATOM	160	CG	GLU	A	78	30.222	37.503	36.974	1.00 24.70
ATOM	161	CD	GLU	A	78	31.225	38.342	37.757	1.00 26.24
MOTA	162		GLU		78	31.162	39.584	37.679	1.00 27.53
MOTA	163		GLU		78	32.076	37.755	38.452	1.00 29.49
MOTA	164	N	MET		79	27.296	37.012	35.641	1.00 16.65
MOTA	165	CA	MET		79	25.992	37.684	35.761	1.00 17.22
MOTA	166	С	MET		79	25.610	37.768	37.232	1.00 17.77
MOTA	167	0	MET	A	79	26.208	37.066	38.100	1.00 18.29
ATOM	168	CB	MET	Α	79	24.908	36.899	35.007	1.00 16.88
ATOM	169	CG	MET	A	79	25.070	36.874	33.492	1.00 16.65
MOTA	170	SD	MET		79	23.798	35.865	32.673	1.00 17.43
MOTA	171	CE	MET		79	22.442	37.003	32.577	1.00 15.55
	172		THR				38.617		1.00 17.73
ATOM		N			80	24.637		37.539	
MOTA	173	CA	THR		80	24.146	38.741	38.917	1.00 17.50
MOTA	174	C	THR		80	22.632	38.630	38.853	1.00 17.85
MOTA	175	0	THR		80	21.995	39.075	37.851	1.00 17.14
MOTA	176	CB	THR	A	80	24.524	40.100	39.550	1.00 18.12
MOTA	177	OG1	THR		80	23.851	41.158	38.857	1.00 18.55
MOTA	178	CG2	THR		80	26.031	40.328	39.474	1.00 16.48
ATOM	179	N	VAL		81	22.042	38.020	39.874	1.00 18.24
ATOM	180	CA	VAL		81	20.573	37.882	39.959	1.00 20.23
	181	C							
MOTA			VAL		81	20.145	38.274	41.375	1.00 21.18
MOTA	182	0	LAV	A	81	20.929	38.093	42.362	1.00 20.31

ATOM	183	СВ	VAL A	81	20.105	36.429	39.700	1.00 20.43
MOTA	184	CG1	. VAL A	81	20.566	35.959	38.334	1.00 21.49
MOTA	185	CG2	VAL A		20.639	35.518	40.777	
MOTA	186	N	GLY A		18.938	38.817	41.497	1.00 21.84
MOTA	187	CA	GLY A		18.421	39.200	42.799	1.00 21.10
MOTA	188	C	GLY A		18.973	40.475	43.404	1.00 21.47
ATOM	189	Ö	GLY A		19.864	41.159	42.814	
MOTA	190	И	SER A		18.454	40.808	44.581	
								1.00 22.27
MOTA	191	CA	SER A		18.869	42.012	45.335	1.00 22.02
MOTA	192	C	SER A		18.996	41.607	46.795	1.00 20.16
MOTA	193	0	SER A		18.002	41.120	47.410	1.00 20.07
MOTA	. 194	CB	SER A		17.804	43.104	45.213	1.00 21.98
MOTA	195	OG	SER A		17.356	43.229	43.874	1.00 23.70
MOTA	196	N	PRO A		20.198	41.734	47.380	1.00 21.14
MOTA	197	CA	PRO A		21.454	42.221	46.785	1.00 20.45
MOTA	198	С	PRO A	84	21.911	41.288	45.656	1.00 20.37
MOTA	199	0	PRO A	84	21.508	40.086	45.606	1.00 18.46
MOTA	200	CB	PRO A	84	22.434	42.193	47.962	1.00 19.74
ATOM	201	CG	PRO A	84	21.548	42.320	49.166	1.00 20.71
MOTA	202	CD	PRO A	84	20.377	41.447	48.815	1.00 19.44
MOTA	203	N	PRO A	85	22.754	41.790	44.741	1.00 20.53
MOTA	204	CA	PRO A	85	· 23.258	40.997	43.616	1.00 20.58
MOTA	205	С	PRO A	85	23.949	39.706	44.046	1.00 20.81
ATOM	206	ō	PRO A	85	24.854	39.720	44.936	1.00 21.15
MOTA	207	ĊВ	PRO A	85	24.240	41.947	42.932	1.00 20.87
ATOM	208	CG	PRO A	85	23.732	43.294	43.282	1.00 22.23
ATOM	209	CD	PRO A	85	23.732	43.141	44.724	1.00 21.41
MOTA	210	N	GLN A	86	23.541	38.590	43.453	1.00 20.05
MOTA	211	CA	GLN A	86	24.174	37.289	43.752	1.00 19.63
MOTA	212	C	GLN A	86	24.174	36.923	42.472	1.00 20.50
MOTA	213	0	GLN A	86				
	213				24.263	36.622	41.412	1.00 19.85
MOTA		CB	GLN A	86	23.127	36.227	44.097	1.00 19.82
ATOM	215	CG	GLN A	86	22.283	36.586	45.314	1.00 18.97
MOTA	216	CD	GLN A	86	21.292	35.506	45.693	1.00 19.84
ATOM	217		GLN A	86	20.226	35.801	46.316	1.00 21.21
MOTA	218		GLN A	86	21.603	34.259	45.354	1.00 17.54
MOTA	219	N	THR A	87	26.229	36.969	42.527	1.00 19.61
MOTA	220	CA	THR A	87	27.057	36.669	41.346	1.00 19.61
MOTA	221	C	THR A	87	27.088	35.188	40.994	1.00 18.63
MOTA	222	0	THR A	87	27.220	34.302	41.892	1.00 18.56
MOTA	223	CB	THR A	87	28.501	37.164	41.549	1.00 19.88
MOTA	224		THR A	87	28.486	38.558	41.887	1.00 20.57
MOTA	225	CG2	THR A	87	29.304	36.977	40.278	1.00 18.65
MOTA	226	N	LEU A	88	26.972	34.907	39.701	1.00 18.38
MOTA	227	CA	LEU A	88	26.991	33.522	39.193	1.00 18.18
ATOM	228	C	LEU A	88	27.572	33.496	37.781	1.00 18.11
MOTA	229	0	LEU A	88	27.353	34.457	36.974	1.00 18.86
ATOM	230	CB	LEU A	88	25.568	32.952	39.159	1.00 16.21
MOTA	231	CG	LEU A	88	24.825	32.828	40.495	1.00 18.20
MOTA	232	CD1	LEU A	88	23.366	32.474	40.226	1.00 18.10
MOTA	233	CD2	LEU A	88	25.484	31.766	41.379	1.00 16.56
MOTA	234	N	ASN A	89	28.317	32.443	37.459	1.00 15.84
ATOM	235	CA	ASN A	89	28.876	32.312	36.101	1.00 16.22
ATOM	236	С	ASN A	89	27.841	31.544	35.300	1.00 16.03
MOTA	237	Ō	ASN A	89	27.363	30.450	35.735	1.00 15.05
MOTA	238	СВ	ASN A	89	30.208	31.565	36.114	1.00 15.71
ATOM	239	CG	ASN A	89	31.324	32.396	36.700	1.00 15.71
MOTA	240		ASN A	89	31.324	33.650	36.477	1.00 15.10
MOTA	241		ASN A	89	32.217	31.750		1.00 13.48
MOTA	242	N	ILE A	90	27.485	32.091	37.439	
ATOM	242	CA					34.145	1.00 15.55
MOTA	244	CA	ILE A	90 90	26.445	31.494	33.292	1.00 14.59
WI OLI	7.4.4	C	THE A	<b>7</b> 0	26.960	31.052	31.930	1.00 15.07

ATOM	245	0	ILE	Α	90	27.578	31.867	31.173	1.00 13.01
ATOM	246	CB	ILE	Α	90	25.301	32.512	33.084	1.00 14.44
ATOM	247	CG1			90	24.884	33.098	34.437	1.00 14.15
	248	CG2			90	24.114	31.847	32.407	1.00 14.29
ATOM									
ATOM	249	CD1			90	24.356	32.062	35.426	1.00 13.44
ATOM	250	N	LEU		91	26.714	29.790	31.590	1.00 15.08
ATOM	251	CA	LEU	Α	91	27.153	29.249	30.284	1.00 15.63
ATOM	252	С	LEU	Α	91	26.313	29.878	29.174	1.00 16.04
ATOM	253	0	LEU	Α	91	25.041	29.904	29.250	1.00 16.72
ATOM	254	CB	LEU		91	27.008	27.721	30.265	1.00 14.67
ATOM	255	CG	LEU		91	27.450	26.945	29.012	1.00 15.49
						27.692	•		
ATOM	256	CD1			91		25.485	29.364	1.00 15.10
ATOM	257	CD2			91	26.393	27.052	27.925	1.00 15.54
MOTA	258	N	VAL		92	26.995	30.408	28.164	1.00 16.13
MOTA	259	CA	VAL	A	92	26.336	31.051	27.003	1.00 15.39
MOTA	260	С	VĄL	Α	92	25.901	29.960	26.038	1.00 15.51
ATOM	261	0	VAL	A	92	26.761	29.243	25.440	1.00 16.92
ATOM	262	СВ	VAL	Α	92	27.306	32.008	26.278	1.00 15.40
ATOM	263		VAL		92	26.668	32.523	24.994	1.00 16.99
ATOM	264	CG2			92	27.671	33.172	27.200	1.00 13.64
ATOM	265	N	ASP		93	24.594	29.824	25.845	1.00 16.41
ATOM	266	CA	ASP		93	24.069	28.762	24.974	1.00 14.41
ATOM	267	C	ASP		93	23.090	29.226	23.903	1.00 15.40
MOTA	268	O	ASP	Α	93	21.889	29.494	24.206	1.00 15.81
MOTA	269	CB	ASP	A	93	23.411	27.701	25.861	1.00 16.00
ATOM	270	CG	ASP	A.	93	22.897	26.512	25.078	1.00 16.45
ATOM	271	OD1	ASP	Α	93	23.536	26.133	24.076	1.00 17.23
ATOM	272		ASP		93	21.863	25.938	25.481	1.00 16.68
ATOM	273	N	THR		94	23.550	29.326	22.657	1.00 13.38
MOTA	274	CA	THR		94	22.636	29.745	21.574	1.00 13.70
						•			
MOTA	275	Ċ	THR		94	21.811	28.549	21.109	1.00 13.68
MOTA	276	0	THR		94	20.941	28.671	20.190	1.00 14.18
ATOM	277	CB	THR	A	94	23.397	30.349	20.362	1.00 14.99
ATOM	278	OG1	THR	Α	94	24.279	29.370	19.798	1.00 14.96
MOTA	279	CG2	THR	Α	94	24.201	31.568	20.794	1.00 14.04
ATOM	280	N	GLY	A	95	22.053	27.392	21.719	1.00 14.90
ATOM	281	CA	GLY	Α	95	21.309	26.199	21.351	1.00 15.51
ATOM	282	C	GLY		95	20.108	25.969	22.255	1.00 16.96
MOTA	283	ō	GLY		95	19.516	24.850	22.275	1.00 16.90
ATOM	284	N	SER		96	19.721	26.987	23.011	1.00 17.38
	285								
ATOM		CA	SER		96	18.562	26.851	23.922	1.00 17.95
MOTA	286	C	SER		96	17.990	28.231	24.226	1.00 17.07
MOTA	287	0	SER		96	18.573	29.269	23.803	1.00 14.94
ATOM	288	CB	SER		96	19.005	26.174	25.219	1.00 18.55
ATOM	289	OG	SER		96	19.640	26.894	26.276	1.00 26.99
MOTA	290	N	SER	A	97	16.869	28.292	24.936	1.00 16.25
ATOM	291	CA	SER	A	97	16.290	29.614	25.258	1.00 18.39
MOTA	292	С	SER		97	15.740	29.776	26.670	1.00 17.83
ATOM	293	0	SER		97	14.866	30.653	26.932	1.00 18.75
MOTA	294	СВ	SER		97	15.224	29.993	24.227	1.00 18.88
	295		SER		97				
ATOM		OG				14.633	28.850	23.651	1.00 23.68
MOTA	296	N	ASN		98	16.229	28.959	27.592	1.00 17.57
MOTA	297	CA	ASN		98	15.809	29.073	28.993	1.00 16.01
MOTA	298	C	ASN	A	98	16.963	29.611	29.821	1.00 16.51
ATOM	299	0	ASN	A	98	18.127	29.109	29.709	1.00 16.69
ATOM	300	CB	ASN	Α	98	15.401	27.720	29.566	1.00 13.74
ATOM	301	CG	ASN		98	13.969	27.359	29.241	1.00 16.04
ATOM	302		ASN		98	13.669	26.795	28.139	1.00 13.27
ATOM	303		ASN		98	13.058	27.680	30.158	1.00 13.26
ATOM	304	N	PHE		99		30.640	30.614	1.00 13.20
	305	CA	PHE		99	16.688			
MOTA						17.710	31.196	31.519	1.00 13.19
ATOM	306	С	PHE	A	99	17.453	30.424	32.812	1.00 13.23

MOTA	307	0	PHE A	99	16.3		66 33.384	1.00 11.00
ATOM	308	CB	PHE A	99	17.4	91 32.6	99 31.722	1.00 13.54
ATOM	309	CG	PHE A	99	18.3	90 33.3	18 32.761	1.00 14.79
ATOM	310	CD1		99	19.7	41 32.9	78 32.836	1.00 15.02
ATOM	311	CD2	PHE A		17.8			
ATOM	312	CE1	PHE A		20.5			
ATOM	313	CE2	PHE A		18.7			
ATOM	314	CZ	PHE A		20.0			
			ALA A		18.4			
ATOM	315	N			18.2			
ATOM	316	CA	ALA A					
ATOM	317	C	ALA A		19.5			
ATOM	318	0	ALA A		20.7			
ATOM	319	CB	ALA A		17.8			
MOTA	320	N	VAL A		19.4			
MOTA	321	CA	VAL A		20.6			
MOTA	322	С	VAL A		20.4			
ATOM	323	0	VAL A		19.2			
ATOM	324	CB	VAL A		20.9	12 30.0		
ATOM	325	CG1	VAL A	101	21.1	26 31.09	98 36.962	1.00 12.49
ATOM	326	CG2	VAL A	101	19.7	43 30.50	09 38.953	1.00 13.11
ATOM	327	N	GLY A	102	21.5	28 27.12	20 39.098	
ATOM	328	CA	GLY A	102	21.4	37 26.18	39 40.207	1.00 17.46
ATOM	329	С	GLY A	102	20.8	58 26.96	56 41.375	1.00 19.61
MOTA	330	0	GLY A	102	21.3	03 28.12	28 41.641	1.00 19.12
ATOM	331	N	ALA A	103	19.8	75 26.39	95 42.065	1.00 19.81
ATOM	332	CA	ALA A	103	19.2			
ATOM	333	C	ALA A		19.0			
ATOM	334	ō	ALA A		18.1			1.00 24.50
ATOM	335	СВ	ALA A		17.8			
ATOM	336	N	ALA A		19.9			1.00 23.53
ATOM	337	CA	ALA A		19.9			1.00 24.47
ATOM	338	C	ALA A		21.3			1.00 24.98
ATOM	339	0	ALA A		21.9			1.00 24.55
ATOM	340	СВ	ALA A		18.8			1.00 23.55
MOTA	341		PRO A		21.8			1.00 25.27
		N	PRO A		23.1			1.00 23.27
MOTA	342	CA	PRO A		23.3			1.00 24.87
MOTA	343	C	PRO A		22.3			1.00 24.16
MOTA	344	O						
MOTA	345	CB	PRO A		23.1			1.00 25.36
MOTA	346	CG	PRO A		22.3			1.00 25.71
ATOM	347	CD	PRO A		21.1			
MOTA	348	N	HIS A		24.5			1.00 24.93
MOTA	349	CA	HIS A		24.9			1.00 23.63
MOTA	350	C	HIS A		26.40			1.00 24.29
MOTA	351	0	HIS A		27.20			1.00 24.19
ATOM	352	CB	HIS A		24.6			1.00 24.15
MOTA	353	CG	HIS A		24.88			1.00 24.43
ATOM	354		HIS A		23.93			1.00 25.53
MOTA	355		HIS A		26.0			1.00 23.79
MOTA	356		HIS A		24.43			1.00 25.66
ATOM	357		HIS A		25.69			1.00 24.92
MOTA	358	N	PRO A	107	26.83		2 44.236	1.00 25.36
MOTA	359	CA	PRO A	107	28.22		0 44.358	1.00 26.23
MOTA	360	C	PRO A		29.1			1.00 26.26
MOTA	361	0	PRO A	107	30.33		6 43.866	1.00 28.01
MOTA	362	CB	PRO A	107	28.22	25 16.72	2 43.972	1.00 26.21
MOTA	363	CG	PRO A	107	26.87	5 16.25	9 44.418	1.00 26.75
MOTA	364	CD	PRO A		25.97			1.00 25.04
ATOM	365	N	PHE A	108	28.69			1.00 25.94
MOTA	366	CA	PHE A		29.55			1.00 26.76
MOTA	367	С	PHE A		29.35			1.00 26.66
MOTA	368	0	PHE A		30.10			1.00 26.81

ATOM	369	CB	PHE A	108	29.368	19.754	39.936	1.00 26.67
ATOM	370	CG	PHE A		29.665	18.300	39.720	1.00 26.80
ATOM	371	CD1			30.531	17.614	40.569	1.00 27.67
ATOM	372	CD2			29.090	17.615	38.655	1.00 27.12
ATOM	373	CE1			30.819	16.262	40.359	1.00 27.99
ATOM	374	CE2	PHE A	108	29.369	16.267	38.433	1.00 26.65
ATOM .	375	CZ	PHE A	108	30.235	15.587	39.286	1.00 26.94
ATOM	376	N	LEU A		28.386	22.180	42.231	1.00 26.14
ATOM	377	CA	LEU A		28.144	23.629	42.346	1.00 27.17
						24.248		
ATOM	378	C	LEU A		28.914		43.510	1.00 29.20
MOTA	379	0	LEU A		28.861	23.743	44.669	1.00 26.91
MOTA	380	CB	LEU A		26.647	23.911	42.498	1.00 25.73
ATOM	381	CG	LEU A	109	25.811	23.714	41.230	1.00 25.94
MOTA	382	CD1	LEU A	109	24.343	23.983	41.530	1.00 24.99
ATOM	383	CD2	LEU A	109	26.310	24.657	40.136	1.00 24.26
ATOM	384	N	HIS A		29.632	25.328	43.213	1.00 32.94
ATOM	385	CA	HIS A		30.442	26.077		1.00 35.82
MOTA	386	C	HIS A		29.533	27.015	44.983	1.00 33.93
ATOM	387	0	HIS A		29.732	27.265	46.209	1.00 34.20
MOTA	388	CB	HIS A		31.501	26.915	43.485	1.00 42.49
ATOM	389	CG	HIS A	110	32.907	26.469	43.732	1.00 47.84
ATOM	390	ND1	HIS A	110	33.509	26.558	44.969	1.00 50.74
ATOM	391	CD2	HIS A	110	33.834	25.934	42.899	1.00 49.74
ATOM	392		HIS A		34.746	26.098	44.888	1.00 51.83
ATOM	393	NE2			34.968	25.713	43.644	1.00 51.38
						27.553		
ATOM	394	N	ARG A		28.547		44.279	1.00 31.13
MOTA	395	CA	ARG A		27.579	28.494	44.857	1.00 28.72
MOTA	396	С	ARG A		26.287	28.331	44.072	1.00 28.16
MOTA	397	0	ARG A	111	26.267	27.652	43.000	1.00 27.40
MOTA	398	CB	ARG A	111	28.108	29.924	44.717	1.00 28.09
ATOM	399	CG	ARG A	111	28.550	30.255	43.305	1,00 26.48
ATOM	400	CD	ARG A		29.216	31.616	43.201	1.00 25.86
ATOM	401	NE	ARG A		29.723	31.831	41.849	1.00 25.21
ATOM	402	CZ	ARG A		30.423	32.892	41.465	1.00 24.44
ATOM	403	NH1			30.708	33.850	42.337	1.00 25.08
ATOM	404	NH2			30.828	32.995	40.205	1.00 22.62
ATOM	405	N	TYR A		25.207	28.922	44.566	1.00 26.27
MOTA	406	CA	TYR A	112	23.922	28.814	43.866	1.00 23.70
MOTA	407	C	TYR A	112	22.955	29.916	44.250	1.00 22.77
MOTA	408	0	TYR A	112	23.140	30.633	45.283	1.00 21.10
ATOM	409	CB	TYR A	112	23.295	27.437	44.119	1.00 25.47
ATOM	410	CG	TYR A		23.036	27.111	45.575	1.00 27.20
ATOM	411	CD1			21.885	27.569	46.222	1.00 28.51
MOTA	412		TYR A		23.946	26.353	46.309	1.00 27.51
MOTA	413		TYR A		21.647	27.276	47.565	1.00 27.78
MOTA	414		TYR A		23.720	26.058	47.651	1.00 28.63
MOTA	415	CZ	TYR A	112	22.570	26.522	48.270	1.00 28.98
MOTA	416	OH	TYR A	112	22.352	26.228	49.591	1.00 30.28
ATOM	417	N	TYR A	113	21.927	30.069	43.428	1.00 19.32
MOTA	418	CA	TYR A		20.896	31.090	43.624	1.00 18.94
MOTA	419	С	TYR A		20.047	30.807	44.857	1.00 17.90
ATOM	420	ō	TYR A		19.480	29.688	45.011	1.00 19.37
								1.00 17.76
MOTA	421	CB	TYR A		20.027	31.141	42.369	
MOTA	422	CG	TYR A		18.887	32.135	42.378	1.00 17.68
MOTA	423		TYR A		19.024	33.397	42.963	1.00 16.86
MOTA	424	CD2	TYR A	113	17.709	31.854	41.688	1.00 16.79
MOTA	425	CE1	TYR A	113	18.020	34.349	42.848	1.00 17.05
MOTA	426		TYR A		16.704	32.796	41.563	1.00 16.02
ATOM	427	CZ	TYR A		16.858	34.038	42.138	1.00 17.36
MOTA	428	ОН	TYR A		15.848	34.963	41.984	1.00 16.62
ATOM	429	N	GLN A		19.967	31.790	45.746	1.00 18.68
ATOM								1.00 20.28
PION	430	CA	GLN A	714	19.156	31.673	46.983	1.00 20.20

ATOM 432 O GLN A 114 18.285 33.933 47.192 1.00 ATOM 433 CB GLN A 114 20.028 31.912 48.216 1.00 ATOM 434 CG GLN A 114 21.048 30.814 48.434 1.00 ATOM 435 CD GLN A 114 21.942 31.063 49.626 1.00 ATOM 436 OE1 GLN A 114 22.708 32.073 49.668 1.00 ATOM 437 NE2 GLN A 114 21.876 30.173 50.606 1.00 ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 15.234 33.837 47.583 1.00 ATOM 442 CB ARG A 115 14.784 35.022 47.546 1.00 ATOM 443 CG ARG A 115 14.550 32.366 45.686 1.00 ATOM 444 CD ARG A 115 14.807 31.953 44.240 1.00 ATOM 445 NE ARG A 115 13.917 30.796 43.824 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 12.514 28.352 43.732 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.323 33.138 48.710 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.718 34.953 50.343 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 14.972 32.691 51.123 1.00	19.59 20.34 19.79 22.79 24.34 26.47 24.49 20.48 21.24 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99 23.86
ATOM 432 O GLN A 114 18.285 33.933 47.192 1.00 ATOM 433 CB GLN A 114 20.028 31.912 48.216 1.00 ATOM 434 CG GLN A 114 21.048 30.814 48.434 1.00 ATOM 435 CD GLN A 114 21.942 31.063 49.626 1.00 ATOM 436 OE1 GLN A 114 22.708 32.073 49.668 1.00 ATOM 437 NE2 GLN A 114 21.876 30.173 50.606 1.00 ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 13.917 30.796 43.824 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.323 33.138 48.710 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.718 34.953 50.343 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 14.972 32.691 51.123 1.00	19.79 22.79 24.34 26.47 24.49 20.48 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 433 CB GLN A 114 20.028 31.912 48.216 1.00 ATOM 434 CG GLN A 114 21.048 30.814 48.434 1.00 ATOM 435 CD GLN A 114 21.942 31.063 49.626 1.00 ATOM 436 OE1 GLN A 114 22.708 32.073 49.668 1.00 ATOM 437 NE2 GLN A 114 21.876 30.173 50.606 1.00 ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 13.917 30.796 43.824 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.718 34.953 50.343 1.00 ATOM 451 C GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00	19.79 22.79 24.34 26.47 24.49 20.48 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 434 CG GLN A 114 21.048 30.814 48.434 1.00 ATOM 435 CD GLN A 114 21.942 31.063 49.626 1.00 ATOM 436 OE1 GLN A 114 22.708 32.073 49.668 1.00 ATOM 437 NE2 GLN A 114 22.876 30.173 50.606 1.00 ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.703 33.159 46.305 1.00 ATOM 441 O ARG A 115 15.234 33.837 47.583 1.00 ATOM 442 CB ARG A 115 14.784 35.022 47.546 1.00 ATOM 443 CG ARG A 115 14.550 32.366 45.686 1.00 ATOM 444 CD ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 13.917 30.796 43.824 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 13.626 28.428 44.448 1.00 ATOM 448 NH2 ARG A 115 12.514 28.352 43.732 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.718 34.953 50.343 1.00 ATOM 451 C GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 14.972 32.691 51.123 1.00	22.79 24.34 26.47 24.49 20.48 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 435 CD GLN A 114 21.942 31.063 49.626 1.00 ATOM 436 OE1 GLN A 114 22.708 32.073 49.668 1.00 ATOM 437 NE2 GLN A 114 21.876 30.173 50.606 1.00 ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.718 34.953 50.343 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 454 CG GLN A 116 14.972 32.691 51.123 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00	24.34 26.47 24.49 20.48 21.24 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 436 OE1 GLN A 114 22.708 32.073 49.668 1.00 ATOM 437 NE2 GLN A 114 21.876 30.173 50.606 1.00 ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 13.917 30.796 43.824 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 13.626 28.428 44.448 1.00 ATOM 448 NH2 ARG A 115 12.514 28.352 43.732 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.323 33.138 48.710 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	26.47 24.49 20.48 21.24 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 436 OE1 GLN A 114 22.708 32.073 49.668 1.00 ATOM 437 NE2 GLN A 114 21.876 30.173 50.606 1.00 ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 13.917 30.796 43.824 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 13.626 28.428 44.448 1.00 ATOM 448 NH2 ARG A 115 12.514 28.352 43.732 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.323 33.138 48.710 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	26.47 24.49 20.48 21.24 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 437 NE2 GLN A 114 21.876 30.173 50.606 1.00 ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 13.917 30.796 43.824 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 13.626 28.428 44.448 1.00 ATOM 448 NH2 ARG A 115 12.514 28.352 43.732 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.718 34.953 50.343 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 14.972 32.691 51.123 1.00	24.49 20.48 21.24 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 438 N ARG A 115 16.876 32.275 46.479 1.00 ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 13.626 28.428 44.448 1.00 ATOM 448 NH2 ARG A 115 12.514 28.352 43.732 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	20.48 21.24 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 439 CA ARG A 115 15.703 33.159 46.305 1.00 ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 13.917 30.796 43.824 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 13.626 28.428 44.448 1.00 ATOM 448 NH2 ARG A 115 12.514 28.352 43.732 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.323 33.138 48.710 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 15.242 35.873 51.080 1.00 ATOM 454 CG GLN A 116 14.972 32.691 51.123 1.00	21.24 21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.323 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 440 C ARG A 115 15.234 33.837 47.583 1.00 ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 15.323 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	21.94 21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 441 O ARG A 115 14.784 35.022 47.546 1.00 ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	21.40 20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 442 CB ARG A 115 14.550 32.366 45.686 1.00 ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	20.21 20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 443 CG ARG A 115 14.807 31.953 44.240 1.00 ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	20.95 20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	20.32 20.45 19.47 20.02 21.63 22.93 24.99
ATOM 444 CD ARG A 115 13.917 30.796 43.824 1.00 ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	20.45 19.47 20.02 21.63 22.93 24.99
ATOM 445 NE ARG A 115 14.305 29.567 44.508 1.00 ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	20.45 19.47 20.02 21.63 22.93 24.99
ATOM 446 CZ ARG A 115 13.626 28.428 44.448 1.00 ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	19.47 20.02 21.63 22.93 24.99
ATOM 447 NH1 ARG A 115 12.514 28.352 43.732 1.00 ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	20.02 21.63 22.93 24.99
ATOM 448 NH2 ARG A 115 14.061 27.366 45.106 1.00 ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	21.63 22.93 24.99
ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	22.93 24.99
ATOM 449 N GLN A 116 15.323 33.138 48.710 1.00 ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	24.99
ATOM 450 CA GLN A 116 14.880 33.723 49.993 1.00 ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	24.99
ATOM 451 C GLN A 116 15.718 34.953 50.343 1.00 ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	
ATOM 452 O GLN A 116 15.242 35.873 51.080 1.00 ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	<i>23.8</i> 0
ATOM 453 CB GLN A 116 14.972 32.691 51.123 1.00 ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	
ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	24.27
ATOM 454 CG GLN A 116 16.391 32.280 51.502 1.00	27.81
	32.89
ATOM 455 CD GLN A 116 16.999 31.257 50.550 1.00	36.05
	36.88
	37.21
ATOM 458 N LEU A 117 16.944 35.006 49.833 1.00	20.91
	20.59
	19.96
•	18.93
	21.68
ATOM 463 CG LEU A 117 19.887 35.224 51.454 1.00	22.49
·	22.63
	22.12
	18.14
	17.08
ATOM 468 C SER A 118 15.150 38.953 47.436 1.00	16.25
ATOM 469 O SER A 118 14.055 38.316 47.347 1.00	16.00
ATOM 470 CB SER A 118 16.519 37.679 45.787 1.00	
ATOM 472 N SER A 119 15.210 40.250 47.711 1.00	
ATOM 473 CA SER A 119 13.991 41.044 47.973 1.00	18.09
ATOM 474 C SER A 119 13.169 41.307 46.714 1.00	17.35
ATOM 475 O SER A 119 11.964 41.669 46.800 1.00	17.62
ATOM 476 CB SER A 119 14.371 42.380 48.618 1.00	
ATOM 477 OG SER A 119 15.158 43.160 47.727 1.00	
ATOM 478 N THR A 120 13.781 41.137 45.546 1.00	18.90
ATOM 479 CA THR A 120 13.075 41.381 44.263 1.00	17.26
ATOM 480 C THR A 120 12.587 40.104 43.594 1.00	17.17
ATOM 482 CB THR A 120 13.980 42.143 43.283 1.00	
ATOM 483 OG1 THR A 120 15.305 41.609 43.355 1.00	
ATOM 484 CG2 THR A 120 14.012 43.630 43.624 1.00	17.37
ATOM 485 N TYR A 121 12.800 38.977 44.257 1.00	
ATOM 486 CA TYR A 121 12.364 37.676 43.715 1.00	
ATOM 487 C TYR A 121 10.841 37.584 43.606 1.00	
ATOM 488 O TYR A 121 10.088 38.028 44.531 1.00	
ATOM 489 CB TYR A 121 12.878 36.547 44.607 1.00	18.32
ATOM 490 CG TYR A 121 12.187 35.225 44.368 1.00	
	21.48
ATOM 492 CD2 TYR A 121 11.268 34.725 45.291 1.00	21.48

ATOM	493	CE1	TYR A	121	11.776	33.280	42.977	1.00 21.33
ATOM	494	CE2			10.608	33.523	45.067	1.00 22.77
		-	TYR A		10.867	32.807	43.908	1.00 23.35
ATOM	495	CZ						
MOTA	496	OH	TYR 2	121	10.206	31.622	43.682	1.00 23.63
ATOM	497	N	ARG A	122	10.365	37.039	42.492	1.00 16.86
ATOM	498	CA	ARG A	122	8.909	36.851	42.281	1.00 16.79
	499	C	ARG A		8.703	35.397	41.890	1.00 17.46
MOTA								
MOTA	500	0	ARG A		9.348	34.884	40.924	1.00 17.88
ATOM	501	CB	ARG A	122	8.384	37.764	41.174	1.00 14.87
MOTA	502	CG	ARG A	122	8.335	39.230	41.548	1.00 14.83
MOTA	503	CD	ARG A		7.895	40.067	40.369	1.00 14.98
			ARG A		7.822	41.481	40.706	1.00 16.19
MOTA	504	NE						
MOTA	505	CZ	ARG A		7.546	42.442	39.833	1.00 16.67
MOTA	506	NH1	ARG A	122	7.316	42.142	38.559	1.00 15.67
ATOM	507	NH2	ARG A	122	7.505	43.704	40.233	1.00 16.38
ATOM	508	N	ASP A		7.836	34.720	42.628	1.00 18.52
					7.538	33.296	42.388	1.00 19.00
ATOM	509	CA	ASP A					
MOTA	510	C	ASP A		6.435	33.147	41.347	1.00 19.87
MOTA	511	0	ASP A	123	5.342	33.757	41.490	1.00 17.59
ATOM	512	СВ	ASP A	123	7.090	32.657	43.702	1.00 19.80
ATOM	513	CG	ASP A		6.841	31.171	43.582	1.00 20.76
						30.615	42.463	1.00 20.41
MOTA	514		ASP A		6.933			
MOTA	515	OD2			6.549	30.559	44.629	1.00 22.50
MOTA	516	N	LEU A	124	6.689	32.359	40.305	1.00 20.70
ATOM	517	CA	LEU A	124	5.672	32.139	39.255	1.00 21.20
ATOM	518	C	LEU A		4.790	30.929	39.562	1.00 21.64
							38.786	1.00 21.17
MOTA	519	0	LEU A		3.832	30.601		
MOTA	520	CB	LEU A		6.343	31.978	37.888	1.00 21.51
ATOM	521	CG	LEU A	124	6.850	33.288	37.270	1.00 22.05
ATOM	522	CD1	LEU A	124	7.617	32.994	35.997	1.00 22.23
ATOM	523	CD2			5.678	34.217	36.983	1.00 21.49
								1.00 22.67
MOTA	524	N	ARG A		5.083	30.252	40.666	
MOTA	525	CA	ARG A	. 125	4.286	29.078	41.085	1.00 25.58
ATOM	526	С	ARG A	125	4.106	28.081	39.944	1.00 26.39
ATOM	527	0	ARG A	125	2.974	27.552	39.719	1.00 26.83
ATOM	528	СВ	ARG A		2.918	29.553	41.593	1.00 26.62
							42.783	1.00 30.02
ATOM	529	CG	ARG A		3.016	30.511		
MOTA	530	CD	ARG A		1.733	31.311	43.002	1.00 32.48
MOTA	531	NE	ARG A	. 125	1.910	32.334	44.034	1.00 36.63
MOTA	532	CZ	ARG A	125	1.049	33.323	44.282	1.00 38.12
MOTA	533		ARG A		-0.070	33.441	43.575	1.00 37.55
	534-		ARG A		1.307	34.202	45.240	1.00 38.11
MOTA								1.00 26.62
MOTA	535	N	LYS A		5 189	27.810		
ATOM	536	CA	LYS A		5.162	2,6.861	38.079	1.00 26.41
ATOM	537	C	LYS A	. 126	6.453	26.063	37.986	1.00 24.61
ATOM	538	0	LYS A	126	7.577	26.624	38.141	1.00 22.46
ATOM	539	СВ	LYS A		4.971	27.605	36.756	1.00 28.55
						27.804		1.00 32.76
ATOM	540	CG	LYS A		3.539		36.326	
ATOM	541	CD	LYS A		3.486	28.380	34.917	1.00 36.53
ATOM	542	CE	LYS A	126	2.048	28.607	34.456	1.00 38.52
MOTA	543	NZ	LYS A	126	1.234	27.355	34.550	1.00 40.78
ATOM	544	N	GLY A		6.326	24.770	37.731	1.00 23.25
							37.598	1.00 22.82
ATOM	545	CA	GLY A		7.504	23.941		
MOTA	546	С	GLY A		7.970	23.995	36.157	1.00 22.77
MOTA	547	0	GLY A	127	7.220	24.487	35.252	1.00 22.00
MOTA	548	N	VAL A		9.184	23.521	35.909	1.00 21.58
ATOM	549	CA	VAL A		9.731	23.511	34.541	1.00 22.39
							34.390	1.00 21.31
MOTA	550	C	VAL A		10.736	22.388		
MOTA	551	0	VAL A		11.547	22.101	35.323	1.00 21.59
MOTA	552	CB	VAL A	128	10.416	24.851	34.180	1.00 21.77
ATOM	553	CG1	VAL A	128	11.572	25.120	35.122	1.00 22.15
ATOM	554		VAL A		10.903	24.809	32.740	1.00 23.66
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ATOM	555	N	TYR	Α	129		10.700	21.744	33.233	1.00 21.64
MOTA	556	CA	TYR				11.598	20.624	32.933	1.00 21.55
MOTA	557	С	TYR				12.298	20.882	31.609	1.00 20.25
MOTA	558	0	TYR				11.635	21.188	30.573	1.00 20.01
MOTA	559	CB	TYR				10.785	19.333	32.841	1.00 23.37
MOTA	560	CG	TYR				11.545	18.164	32.271	1.00 26.64
ATOM	561		TYR				12.628	17.613	32.956	1.00 27.70
MOTA	562	CD2	TYR				11.178	17.598	31.048	1.00 27.27
ATOM	563	CE1	TYR				13.323	16.529	32.443	1.00 29.33 1.00 28.75
ATOM	564	CE2	TYR				11.872	16.507	30.524	1.00 28.75
ATOM	565	CZ	TYR				12.942	15.980	31.231 30.751	1.00 28.91
ATOM ATOM	566 567	OH	TYR VAL				13.634 13.620	14.896 20.782	31.602	1.00 30.21
ATOM	568	N CA	VAL				14.353	21.003	30.350	1.00 17.21
ATOM	569	C	VAL				15.308	19.872	30.022	1.00 16.02
ATOM	570	Ö	VAL				16.319	19.628	30.748	1.00 16.89
ATOM	571	СВ	VAL				15.136	22.334	30.370	1.00 17.86
ATOM	572		VAL				15.934	22.485	29.075	1.00 15.31
ATOM	573		VAL				14.163	23.505	30.525	1.00 15.67
MOTA	574	N .	PRO	Α	131		15.013	19.136	28.945	1.00 14.83
ATOM	575	CA	PRO	A	131		15.868	18.028	28.529	1.00 14.77
ATOM	576	С	PRO	A	131		16.743	18.516	27.372	1.00 15.00
MOTA	577	0	PRO	Α	131		16.234	19.154	26.402	1.00 15.43
ATOM	578	CB	PRO				14.857	16.971	28.106	1.00 13.57
ATOM	579	CG	PRO				13.809	17.806	27.421	1.00 13.44
ATOM	580	CD	PRO				13.706	19.078	28.262	1.00 13.99
ATOM	581	N	TYR				18.043	18,268	27.465	1.00 14.75
ATOM	582	CA	TYR				18.989	18.679	26.404	1.00 17.37
ATOM	583	C	TYR				19.438	17.415	25.676	1.00 17.52
ATOM	584	O	TYR TYR				19.100 20.211	16.274 19.369	26.105 27.020	1.00 17.41 1.00 16.93
ATOM	585 586	CB CG	TYR			•	19.909	20.665	27.742	1.00 10.93
ATOM ATOM	587		TYR				19.834	21.881	27.051	1.00 17.88
ATOM	588		TYR				19.706	20.681	29.122	1.00 19.01
ATOM	589		TYR				19.564	23.080	27.722	1.00 16.57
ATOM	590		TYR				19.435	21.867	29.799	1.00 17.74
ATOM	591	CZ	TYR				19.365	23.062	29.098	1.00 19.02
ATOM	592	OH	TYR				19.083	24.229	29.782	1.00 18.23
MOTA	593	N	THR				20.188	17.574	24.592	1.00 18.46
MOTA	594	CA	THR	A	133		20.686	16.403	23.842	1.00 18.54
MOTA	595	C	THR	A	133		21.525	15.580	24.812	1.00 20.42
MOTA	596	0	THR				21.667	14.325	24.672	1.00 19.49
MOTA	597		THR				21.546	16.846	22.653	1.00 18.40
MOTA	598		THR				20.720	17.539	21.708	1.00 20.46
MOTA	599		THR			•	22.194	15.645	21.976	1.00 18.37
ATOM	600		GLN .				22.064	16.265	25.810	1.00 22.23
ATOM	601		GLN .				22.890	15.624	26.842	1.00 24.27
MOTA	602		GLN .				22.723	16.406	28.140 28.252	1.00 23.32
ATOM	603 604		GLN .				23.179	17.580	26.405	1.00 21.03 1.00 28.22
ATOM ATOM	605		GLN .				24.352 25.140	15.633 14.412	26.808	1.00 28.22
ATOM	606		GLN .				25.020	13.296	25.781	1.00 32.70
ATOM	607		GLN .				26.052	12.680	25.356	1.00 37.34
ATOM	608		GLN .				23.791	13.018	25.350	1.00 38.92
ATOM	609		GLY .				22.080	15.789	29.124	1.00 23.28
MOTA	610		GLY .				21.863	16.460	30.391	1.00 21.50
ATOM	611		GLY .				20.432	16.946	30.483	1.00 22.11
ATOM	612		GLY .				19.735	17.111	29.435	1.00 20.68
ATOM			LYS :	A.	136		19.968	17.190	31.703	1.00 22.97
MOTA			LYS :				18.584	17.654	31.923	1.00 23.80
MOTA	615		LYS 3				18.429	18.147	33.353	1.00 22.33
ATOM	616	0	LYS 3	A	136		19.196	17.719	34.269	1.00 21.42

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MOTA	617	CB	LYS	Α	136		17.606	16.501	31.677	1.00 25.37
ATOM	618	CG	LYS	Α	136		17.823	15.310	32.607	1.00 28.29
MOTA	619	CD			136		16.804	14.196	32.374	1.00 31.54
MOTA	620	-					16.955			
		CE			136			13.570	31.000	1.00 34.21
MOTA	621	NZ			136		15.996	12.444	30.789	1.00 37.76
MOTA	622	N	TRP	Α	137		17.470	19.040	33.573	1.00 21.02
MOTA	623	CA	TRP	Α	137		17.214	19.562	34.928	1.00 20.75
ATOM	624	С	TRP	Α	137		15.750	19.907	35.133	1.00 20.62
ATOM	625	ō			137		14.951	19.978	34.153	1.00 20.05
ATOM	626	СВ			137		18.077	20.800	35.231	1.00 18.46
MOTA	627	CG			137		17.960	21.937	34.248	1.00 18.02
MOTA	628	CD1			137		18.865	22.276	33.281	1.00 18.12
MOTA	629	CD2		Α	137		16.881	22.879	34.134	1.00 17.27
MOTA	630	NE1	TRP	Α	137		18.419	23.369	32.574	1.00 17.78
ATOM	631	CE2	TRP	Α	137		17.204	23.758	33.074	1.00 17.40
ATOM	632	CE3	TRP	Α	137		15.675	23.067	34.823	1.00 17.08
ATOM	633	CZ2			137		16.363	24.807	32.684	1.00 15.50
ATOM	634	CZ3			137		14.836	24.113	34.434	1.00 17.23
		CH2				٠				
MOTA	635				137		15.188	24.968	33.373	1.00 17.46
MOTA	636	N			138		15.385	20.098	36.395	1.00 21.53
ATOM	637	CA			138		14.014	20.472	36.789	1.00 24.94
MOTA	638	C	GLU	Α	138		14.166	21.642	37.745	1.00 23.18
ATOM	639	0	GLU	Α	138		15.168	21.719	38.526	1.00 21.21
MOTA	640	CB	GLU	Α	138		13.320	19.320	37.515	1.00 28.46
ATOM	641	CG	GLU	Α	138		13.053	18.101	36.656	1.00 34.91
ATOM	642	CD			138		12.562	16.919	37.472	1.00 37.93
ATOM	643	OE1								
							12.175	15.897	36.864	1.00 40.28
ATOM	644	OE2					12.570	17.009	38.722	1.00 40.20
MOTA	645	N	GLY				13.214	22.559	37.711	1.00 22.13
MOTA	646	CA	GLY	A	139		13.298	23.693	38.604	1.00 22.60
MOTA	647	C	GLY	Α	139		11.975	24.402	38.713	1.00 21.54
MOTA	648	0	GLY	Α	139		10.949	23.953	38.116	1.00 23.29
ATOM	649	N	GĽΰ	Α	140		11.962	25.494	39.465	1.00 21.74
ATOM	650	CA	GLU				10.733	26.284	39.648	1.00 21.81
ATOM	651	C	GLU				10.900	27.646	38.998	
ATOM	652				140		11.975			1.00 19.04
		0				•		28.304	39.125	1.00 18.42
ATOM	653	CB	GLU				10.404	26.425	41.139	1.00 24.39
ATOM	654	CG	GLU				11.479	25.887	42.065	1.00 28.61
MOTA	655	CD	GLU	A	140		10.922	25.385	43.383	1.00 29.72
ATOM	656	OE1	${ t GLU}$	Α	140		10.311	24.297	43.389	1.00 31.43
MOTA	657	OE2	GLU	Α	140		11.091	26.077	44.410	1.00 30.48
ATOM	658	N	LEU	Α	141		9.870	28.071	38.278	1.00 16.35
MOTA	659	CA	LEU				9.901	29.360	37.585	
ATOM	660	С	LEU				9.674	30.546	38.511	1.00 15.68
ATOM	661	Õ	LEU				8.832	30.499	39.466	
										1.00 13.45
MOTA	662		LEU				8.864	29.376	36.460	1.00 15.23
MOTA	663	CG	LEU				9.145	28.412	35.300	1.00 16.27
MOTA	664		LEU				8.008	28.461	34.300	1.00 15.60
MOTA	665	CD2	LEU	A	141		10.458	28.785	34.627	1.00 16.48
ATOM	666	N	$\mathtt{GLY}$	Α	142		10.424	31.608	38.241	1.00 15.15
MOTA	667	CA	GLY	Α	142		10.323	32.819	39.015	1.00 12.33
MOTA	668	С	GLY				10.845	33.953	38.167	1.00 14.67
MOTA	669	Ō	GLY				11.242	33.758	36.971	1.00 13.75
ATOM	670	N					10.877			
			THR					35.137	38.754	1.00 14.88
ATOM	671	CA	THR				11.354	36.324	38.050	1.00 15.26
MOTA	672	C	THR				12.262	37.103	39.008	1.00 14.53
MOTA	673	0	THR				12.119	36.991	40.269	1.00 13.46
MOTA	674	CB	THR				10.131	37.154	37.600	1.00 16.18
ATOM	675	OG1	THR	Α	143		10.192	37.362	36.187	1.00 20.69
MOTA	676		THR				10.058	38.465	38.325	1.00 12.43
ATOM	677	N	ASP				13.202	37.866	38.466	1.00 14.22
ATOM	678	CA	ASP				14.117	38.652	39.321	1.00 15.38
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MOTA	679	С	ASP			14.942	39.609	38.479	1.00 15.67
MOTA	680	0	ASP			14.984	39.496	37.208	1.00 16.83
MOTA	681	CB	ASP			15.063	37.721	40.086	1.00 15.20
MOTA	682	CG	ASP			15.367	38.218	41.496	1.00 17.84
MOTA	683		ASP			15.359	39.447	41.724	1.00 16.62
MOTA	684		ASP			15.630	37.373	42.379	1.00 16.33
MOTA	685	N	LEU			15.596	40.551	39.147	1.00 16.74
MOTA	686	CA	LEU			16.442	41.537	38.454	1.00 18.66
MOTA	687	C	LEU			17.757	40.854	38.101	1.00 20.21
MOTA	688	0	LEU			18.381	40.147	38.961	1.00 21.75
ATOM	689	CB	LEU			16.697	42.746	39.351	1.00 18.43
MOTA	690	CG	LEU			15.452	43.522	39.786	1.00 19.69
MOTA	691		LEU			15.878 14.660	44.720 43.971	40.628 38.557	1.00 19.11 1.00 18.50
ATOM ATOM	692	CD2	VAL			18.186	41.030	36.858	1.00 18.30
ATOM	693 694	CA	VAL			19.426	40.402	36.387	1.00 20.48
ATOM	695	CA	VAL			20.331	41.426	35.725	1.00 22.80
ATOM	696	0	VAL			19.849	42.386	35.725	1.00 22.16
ATOM	697	СВ	VAL			19.118	39.265	35.373	1.00 20.39
ATOM	698	CG1	VAL			20.405	38.575	34.941	1.00 20.39
ATOM	699		VAL .			18.163	38.261	35.998	1.00 17.90
ATOM	700	N	SER			21.633	41.251	35.913	1.00 22.35
ATOM	701	CA	SER			22.615	42.158	35.309	1.00 23.39
ATOM	702	C	SER			23.829	41.383	34.833	1.00 21.77
ATOM	703	0	SER			24.119	40.242	35.321	1.00 20.08
MOTA	704	СВ	SER			23.059	43.225	36.316	1.00 25.41
ATOM	705	OG	SER	Α	147	21.993	44.107	36.627	1.00 31.97
MOTA	706	N	ILE .	A	148	24.534	41.972	33.878	1.00 19.69
MOTA	707	CA	ILE .	Α	148	25.757	41.377	33.329	1.00 19.14
MOTA	708	C	ILE .	Α	148	26.853	42.405	33.614	1.00 18.85
MOTA	709	0	ILE .	A	148	27.021	43.408	32.853	1.00 17.87
MOTA	710	CB	ILE .			25.618	41.137	31.817	1.00 18.61
MOTA	711	CG1	ILE .			24.449	40.181	31.559	1.00 19.01
MOTA	712	CG2	ILE .			26.909	40.564	31.255	1.00 17.68
ATOM	713	CD1	ILE .			24.221	39.864	30.097	1.00 19.61
MOTA	714	N	PRO .			27.601	42.214	34.711	1.00 17.99
ATOM	715	CA	PRO .			28.679	43.134	35.095	1.00 21.17
ATOM	716	C	PRO .			29.523	43.638	33.926	1.00 22.18
ATOM ATOM	717 718	O CB	PRO .			29.800 29.485	44.869 42.317	33.823 36.103	1.00 24.08 1.00 19.87
ATOM	719	CG	PRO :			28.404	41.529	36.797	1.00 19.57
MOTA	720	CD	PRO 2			27.542	41.061	35.628	1.00 17.55
ATOM	721	N	HIS !			29.930	42.733	33.041	1.00 23.43
ATOM	722	CA	HIS I			30.748	43.119	31.869	1.00 23.84
ATOM	723	C	HIS			29.933	43.067	30.588	1.00 24.47
ATOM	724	0	HIS 2			30.334	42.431	29.566	1.00 25.89
MOTA	725	СВ	HIS :			31.968	42.211	31.765	1.00 23.54
ATOM	726	CG	HIS I			32.880	42.313	32.945	1.00 26.15
ATOM	727	ND1	HIS 3	A	150	33.619	43.446	33.216	1.00 27.28
ATOM	728		HIS 2			33.149	41.439	33.943	1.00 26.32
MOTA	729		HIS :			34.305	43.264	34.330	1.00 27.48
ATOM	730		HIS :			34.038	42.055	34.791	1.00 28.01
ATOM	731	N	GLY :			28.785	43.727	30.630	1.00 25.49
ATOM	732	CA	GLY :			27.906	43.784	29.485	1.00 26.41
ATOM	733	C	GLY 2			27.325	45.179	29.468	1.00 27.16
ATOM	734	0	GLY 2			27.981	46.136	29.983	1.00 26.97
MOTA	735	N	PRO 3			26.125	45.370	28.903	1.00 28.12
MOTA	736	CA	PRO 2			25.540	46.712	28.880	1.00 28.75
MOTA	737 738	С 0	PRO 2			25.219	47.165	30.304	1.00 30.53 1.00 28.62
MOTA MOTA	738 739	CB	PRO I			24.844 24.294	46.331 46.528	31.182 28.017	1.00 28.62
ATOM	740	CG	PRO 2			23.897	45.105	28.303	1.00 29.49
212 OF1	1-20					23.031	4J.1VJ	20.505	vv 22.03

ATOM	741	CD	PRO A	152		25.227	44.385	28.277	1.00 28.15
ATOM	742	N	ASN A			25.375		30.560	1.00 33.03
MOTA	743	CA	ASN A			25.111		31.902	1.00 34.39
MOTA	744	C	ASN A	153		23.604	49.096	32.144	1.00 33.81
MOTA	745	0	ASN A			23.009	50.218	32.222	1.00 33.63
ATOM	746	СВ	ASN A			25.755	50.401	32.009	1.00 37.16
ATOM	747	CG	ASN A			25.680	50.978	33.406	1.00 38.88
MOTA	748		ASN A		•	25:974	50.272	34.416	1.00 40.17
ATOM	749		ASN A			25.309	52.251	33.504	1.00 39.91
ATOM	750	N	VAL A			22.971	47.934	32.265	1.00 31.55
ATOM	751	CA	VAL A			21.514	47.872	32.486	1.00 29.59
ATOM	752	C	VAL A			21.113	46.739	33.418	1.00 29.47
ATOM	753	ō	VAL A	_		21.924	45.809	33.718	1.00 30.24
ATOM	754	СВ	VAL A			20.755	47.681	31.154	1.00 29.95
MOTA	755		VAL A			20.990	48.875	30.242	1.00 29.70
MOTA	756		VAL A			21.216	46.397	30.474	1.00 28.94
ATOM	757	N	THR A			19.874	46.799	33.882	1.00 27.83
ATOM	758	CA	THR A			19.323	45.773	34.779	1.00 27.61
MOTA	759	С	THR A	155		17.918	45.472	34.296	1.00 26.01
ATOM	760	0	THR A	155		17.114	46.413	34.041	1.00 27.70
MOTA	761	CB	THR A	155		19.268	46.280	36.229	1.00 27.24
MOTA	762	OG1	THR A	155		20.603	46.486	36.703	1.00 29.54
MOTA	763	CG2	THR A	155		18.573	45.270	37.129	1.00 27.37
MOTA	764	N	VAL A	156		17.592	44.197	34.143	1.00 24.69
ATOM	765	CA	VAL A	156		16.241	43.847	33.672	1.00 24.32
MOTA	766	C	VAL A	156		15.631	42.736	34.504	1.00 23.23
MOTA	767	0	VAL A			16.364	41.920	35.154	1.00 23.57
ATOM '	768	CB	VAĻ A			16.253	43.402	32.184	1.00 25.34
ATOM	769		VAL A			17.178	44.302	31,379	1.00 26.63
ATOM	770	CG2				16.684	41.960	32.063	1.00 24.89
ATOM	771	N.	ARG A			14.306	42.687	34.521	1.00 21.44
MOTA	772	CA	ARG A			13.613	41.626	35.262	1.00 20.90
MOTA	773		ARG A		_	13.374	40.560	34.215	1.00 20.13
ATOM	774	0	ARG A	•		12.746	40.836	33.152	1.00 19.99
ATOM	775	CB	ARG A			12.280	42.121	35.830	1.00 20.03
ATOM	776	CG	ARG A		-	11.528	41.053	36.621	1.00 18.95
ATOM	777	CD	ARG A			10.271	41.616	37.260	1.00 18.99
ATOM	778	NE	ARG A			10.554	42.408	38.456	1.00 18.47
ATOM ATOM	779 780	CZ	ARG A			10.973	41.902	39.613	1.00 19.19
ATOM	781	NH1 NH2	ARG A			11.167	40.596	39.747	1.00 18.30
ATOM	782	N	ALA A			11.178 13.878	42.703 39.359	40.650 34.463	1.00 15.82 1.00 20.27
ATOM	783	CA				13.713		33.496	
ATOM	784	C	ALA A			13.713	36.286	34.175	1.00 19.05
ATOM	785	Õ	ALA A			13.379	36.845	35.432	1.00 19.43
ATOM	786	СВ	ALA A			15.017	38.031	32.756	1.00 18.56
ATOM	787	N	ASN A			12.792	36.053	33.370	1.00 18.08
ATOM	788	CA	ASN A			12.363	34.756	33.876	1.00 18.21
ATOM	789	C	ASN A			13.607	33.992	34.282	1.00 18.60
MOTA	790	0	ASN A			14.666	34.033	33.577	1.00 19.42
ATOM	791	CB	ASN A			11.601	33.992	32.797	1.00 16.91
ATOM	792	CG	ASN A			10.282	34.647	32.459	1.00 18.46
ATOM	793		ASN A		•	9.479	34.978	33.381	1.00 19.46
ATOM	794		ASN A			10.020	34.848	31.174	1.00 16.51
MOTA	795	N	ILE A			13.518		35.412	1.00 18.73
MOTA	796	CA	ILE A	160		14.643	32.529	35.916	1.00 17.64
ATOM	797	С	ILE A			14.112	31.191	36.373	1.00 19.09
MOTA	798	0	ILE A	160		13.122	31.125	37.176	1.00 18.38
MOTA	799	CB	ILE A	160		15.319		37.128	1.00 18.36
MOTA	800	CG1	ILE A	160		15.764	34.629	36.758	1.00 17.90
MOTA	801		ILE A			16.521		37.585	1.00 17.16
MOTA	802	CD1	ILE A	160		16.521	35.336	37.875	1.00 18.56

MOTA	803	N	ALA A	161	14.717	30.123	35.871	1.00 17.55
MOTA	804	CA	ALA A		14.314	28.778	36.275	1.00 18.11
MOTA	805	C	ALA A		15.267.	28.394	37.399	1.00 18.26
MOTA	806	0	ALA A		16.507	28.223	37.166	1.00 17.61
MOTA MOTA	807	CB	ALA A		14.447 14.737	27.805	35.105	1.00 17.28
ATOM	808 809	N CA	ALA A		15.567	28.283 27.901	38.614 39.775	1.00 17.99 1.00 18.02
MOTA	810	C	ALA A		15.746	26.382	39.774	1.00 18.02
MOTA	811	ŏ	ALA A		14.835	25.619	40.207	1.00 18.43
ATOM	812	СВ	ALA A		14.897	28.359	41.067	1.00 17.36
ATOM	813	N	ILE A	163	16.900	25.928	39.300	1.00 19.89
MOTA	814	CA	ILE A		17.204	24.480	39.215	1.00 18.56
ATOM	815	C	ILE A		17.314	23.802	40.577	1.00 20.34
ATOM	816	0	ILE A		18.238	24.122	41.402	1.00 19.83
ATOM	817	CB	ILE A		18.512	24.245	38.430	1.00 17.19
ATOM ATOM	818 819	CG1 CG2			18.347 18.874	24.753	36.994	1.00 16.02
ATOM	820	CD1			19.628	22.761 24.735	38.445 36.174	1.00 14.93 1.00 16.24
ATOM	821	N	THR A		16.409	22.860	40.826	1.00 10.24
ATOM	822	CA	THR A		16.379	22.122	42.112	1.00 23.01
MOTA	823	С	THR A	164	16.817	20.665	41.958	1.00 24.30
MOTA	824	0	THR A	164	17.119	19.966	42.973	1.00 26.25
MOTA	825	CB	THR A		14.966	22.173	42.735	1.00 22.01
MOTA	826	OG1			13.990	21.799	41.754	1.00 22.15
MOTA	827	CG2			14.656	23.584	43.214	1.00 22.73
ATOM ATOM	828 829	N CA	GLU A		16.858 17.281	20.187 18.804	40.721 40.444	1.00 25.84
ATOM	830	C	GLU A		17.281	18.693	39.024	1.00 27.82 1.00 26.80
ATOM	831	Ö	GLU A		17.246	19.323	38.072	1.00 26.59
MOTA	832	СВ	GLU A		16.121	17.834	40.678	1.00 31.67
MOTA	833	CG	GLU A	165	16.233	17.118	42.020	1.00 38.94
MOTA	834	CD	GLU A	165	14.913	16.568	42.519	1.00 41.54
ATOM	835		GLU A		14.282	15.765	41.796	1.00 44.35
ATOM	836	OE2			14.510	16.940	43.644	1.00 43.84
ATOM ATOM	837	N	SER A		18.861	17.919	38.852	1.00 24.81
ATOM	838 839	CA C	SER A SER A		19.455 20.213	17.765 16.459	37.525 37.397	1.00 25.32 1.00 25.44
MOTA	840	0	SER A		20.551	15.795	38.427	1.00 23.44
ATOM	841	СВ	SER A		20.405	18.928	37.255	1.00 23.13
MOTA	842	OG	SER A		21.444	18.939	38.217	1.00 21.22
ATOM	843	N	ASP A		20.490	16.079	36.155	1.00 26.01
MOTA	844	CA	ASP A		21.227	14.842	35.871	1.00 26.62
ATOM	845	C	ASP A		22.138			
ATOM ATOM	846 847	O CB	ASP A		21.656	15.300	33.528	1.00 24.35
ATOM	848	CG	ASP A		20.253 20.966	13.691 12.370	35.601 35.387	1.00 30,53 1.00 32.67
ATOM	849		ASP A		21.912	12.083	36.152	1.00 32.07
ATOM	850		ASP A		20.586	11.615	34.469	1.00 34.63
ATOM	851	N	LYS A		23.440	14.930	34.910	1.00 25.32
ATOM	852	CA	LYS A	168	24.461	15.078	33.847	1.00 25.94
ATOM	853	C	LYS A	168	24.416	16.445	33.175	1.00 25.49
ATOM	854	0	LYS A		24.742	16.580	31.955	1.00 25.50
ATOM	855	CB	LYS A		24.282	13.979	32.800	1.00 27.68
ATOM ATOM	856 857	CD	LYS A		24.408	12.570	33.362	1.00 30.33
ATOM ATOM	858	CE	LYS A		24.117 24.205	11.532	32.292	1.00 32.36 1.00 34.37
ATOM	859	NZ	LYS A			10.126 9.101	32.855 31.821	1.00 34.37
ATOM	860	N	PHE A		24.024	17.460	33.937	1.00 30.30
MOTA	861	CA	PHE A		23.942	18.835	33.418	1.00 20.96
MOTA	862	C	PHE A	169	25.158	19.616	33.897	1.00 22.06
MOTA	863	0	PHE A		25.983	20.119	33.069	1.00 20.71
MOTA	864	CB	PHE A	169	22.668	19.506	33.919	1.00 19.76

ATOM	865	CG PHE A 169	22.526	5 20.931	33.479	1.00 18.95
ATOM	866		22.400			
ATOM	867		22.525			
MOTA	868		22.275			
MOTA	869		22.401			
ATOM	870		22.275			
ATOM	871		25.292			
ATOM	872					
			26.438			
ATOM	873		27.702			
ATOM	874		27.675			
ATOM	875		26.205			
ATOM.	876		25.079			
ATOM	877		23.988			1.00 18.45
ATOM	878		25.098			1.00 16.73
ATOM	879		22.932	22.154	38.563	1.00 17.50
MOTA	880	CE2 PHE A 170	24.046	23.832	37.253	1.00 17.78
MOTA	881		22.963	23.432	38.023	1.00 16.39
MOTA	882	N ILE A 171	28.805	20.297	35.272	
ATOM	883	CA ILE A 171	30.095	19.615	35.043	
ATOM	884	C ILE A 171	31.057	19.962	36.163	
ATOM	885	O ILE A 171	31.222	21.162	36.537	
ATOM	886	CB ILE A 171	30.729		33.704	
MOTA	887	CG1 ILE A 171	29.823	19.632	32.544	
ATOM	888	CG2 ILE A 171	32.123	19.434	33.558	
ATOM	889	CD1 ILE A 171	30.319	20.100	31.192	1.00 23.46
ATOM	890	N ASN A 172		18.942	36.709	
ATOM	891	CA ASN A 172	32.657	19.143	37.809	1.00 30.01
ATOM	892	C ASN A 172	33.864	19.975	37.359	1.00 30.01
ATOM	893	O ASN A 172	34.616	19.574	36.418	
ATOM	894	CB ASN A 172	33.105	17.779	38.337	1.00 29.20 1.00 31.92
ATOM	895	CG ASN A 172	33.913	17.773		
MOTA	896	OD1 ASN A 172			39.608	1.00 34.74
ATOM	897	ND2 ASN A 172	33.615	18.737	40.504	1.00 36.04
ATOM	898		34.927	17.034	39.734	1.00 36.14
ATOM		N GLY A 173	34.049	21.132	37.991	1.00 28.24
ATOM	899 900	CA GLY A 173	35.166	22.001	37.659	1.00 27.99
ATOM		C GLY A 173	34.973	22.938	36.476	1.00 28.87
	901	O GLY A 173	35.944	23.644	36.063	1.00 29.20
ATOM ATOM	902	N SER A 174	33.769	22.988	35.914	1.00 28.95
ATOM	903	CA SER A 174	33.498	23.880	34.748	1.00 29.13
	904	C SER A 174	33.524	25.348	35.168	1.00 27.92
MOTA	905	O SER A 174	33.878	26.255	34.354	1.00 29.51
MOTA	906	CB SER A 174	32.130	23.562	34.148	1.00 28.90
MOTA	907	OG SER A 174	31.102	23.922		1.00 30.49
ATOM	908	N ASN A 175	33.140	25.593	36.416	1.00 25.45
MOTA	909	CA ASN A 175	33.095		37.011	1.00 23.59
MOTA	910	C ASN A 175	31.855	27.767	36.647	1.00 21.71
MOTA	911	O ASN A 175	31.828	29.019	36.853	1.00 20.11
MOTA	912	CB ASN A 175	34.354	27.754	36.662	1.00 27.01
MOTA	913	CG ASN A 175	34.548	28.950	37.582	1.00 29.09
MOTA	914	OD1 ASN A 175	34.648	28.794	38.840	1.00 30.19
ATOM	915	ND2 ASN A 175	34.600	30.144	37.004	1.00 30.01
MOTA	916	N TRP A 176	30.841	27.121	36.078	1.00 16.70
ATOM	917	CA TRP A 176	29.590	27.847	35.790	1.00 18.41
MOTA	918	C TRP A 176	28.482	27.170	36.580	1.00 17.87
MOTA	919	O TRP A 176	28.534	25.927	36.838	1.00 15.45
MOTA	920	CB TRP A 176	29.248	27.888	34.292	1.00 16.48
ATOM	921	CG TRP A 176	29.257	26.588	33.563	1.00 17.63
MOTA	922	CD1 TRP A 176	30.291	26.063	32.842	1.00 17.33
ATOM	923	CD2 TRP A 176	28.165	25.668	33.425	1.00 17.78
MOTA	924	NE1 TRP A 176	29.911	24.881	32.258	1.00 16.01
MOTA	925	CE2 TRP A 176	28.612	24.613	32.599	1.00 16.95
MOTA	926	CE3 TRP A 176	26.852	25.635	33.918	1.00 18.29
				:000	55.510	1.00 10.22

MOTA	927	CZ2	TRP A 176	27.794	23.532	32.252	1.00 17.40
ATOM	928	CZ3	TRP A 176	26.034	24.557	33.573	1.00 19.02
MOTA	929	CH2	TRP A 176	26.512	23.521	32.747	1.00 19.06
ATOM	930		. GLU A 177		27.950	37.005	1.00 18.68
MOTA	931	CA	GLU A 177		27.385	37.797	1.00 21.01
ATOM	932	C	GLU A 177		27.700	37.224	1.00 20.81
ATOM	933	Ö	GLU A 177		27.582	37.938	1.00 21.08
	934		GLU A 177			39.250	1.00 22.84
ATOM		CB			27.869		
ATOM	935	CG	GLU A 177		29.322	39.443	1.00 26.63
ATOM	936	CD	GLU A 177		29.531	39.446	1.00 27.90
MOTA	937	OE1			28.568	39.726	1.00 28.44
MOTA	938	OE2			30.670	39.186	1.00 28.24
MOTA	939	N	GLY A 178		28.088	35.953	1.00 18.48
MOTA	940	CA	GLY A 178		28.411	35.295	1.00 16.82
MOTA	941	С	GLY A 178		28.406	33.791	1.00 15.90
MOTA	942	0	GLY A 178		28.248	33.264	1.00 15.75
MOTA	943	N	ILE A 179		28.589	33.076	1.00 14.53
MOTA	944	CA	ILE A 179		28.588	31.610	1.00 14.26
MOTA	945	C	ILE A 179		29.701	31.057	1.00 14.53
MOTA	946	0	ILE A 179		29.980	31.603	1.00 15.23
MOTA	947	CB	ILE A 179		27.217	31.069	1.00 14.45
MOTA	948	CG1	ILE A 179	22.535	27.183	29.548	1.00 14.28
MOTA	949	CG2	ILE A 179	21.002	26.921	31.525	1.00 13.41
MOTA	950	CD1	ILE A 179	22.359	25.788	28.974	1.00 13.85
MOTA	951	N	LEU A 180	22.489	30.350	29.998	1.00 14.91
MOTA	952	CA	LEU A 180	21.763	31.464	29.353	1.00 14.24
MOTA	953	С	LEU A 180	21.311	31.050	27.961	1.00 15.19
ATOM	954	0	LEU A 180	22.117	31.115	26.973	1.00 15.79
MOTA	955	CB	LEU A 180	22.675	32.690	29.223	1.00 14.83
MOTA	956	CG	LEU A 180	22.078	34.107	29.257	1.00 16.59
MOTA	957	CD1	LEU A 180	22.902	34.996	28.351	1.00 15.04
ATOM	958	CD2	LEU A 180	20.622	34.120	28.818	1.00 17.08
ATOM	959	N	GLY A 181		30.621	27.851	1.00 15.40
ATOM	960	CA	GLY A 181	19.525	30.227	26.561	1.00 13.68
ATOM	961	С	GLY A 181		31.481	25.741	1.00 15.03
ATOM	962	0	GLY A 181	18.402	32.330	26.107	1.00 14.58
ATOM	963	N·	LEU A 182	20.002	31.629	24.638	1.00 12.84
MOTA	964	CA	LEU A 182	19.859	32.831	23.787	1.00 13.53
MOTA	965	С	LEU A 182	19.029	32.646	22.521	1.00 14.25
ATOM	966	0	LEU A 182	18.883	33.607	21.701	1.00 13.52
ATOM	967	СВ	LEU A 182	21.250	33.352	23.418	1.00 13.44
ATOM	968	CG	LEU A 182	22.036	33.949	24.583	1.00 11.84
MOTA	969		LEU A 182	23.506			
MOTA	970		LEU A 182	21.450	35.311	24.936	1.00 12.14
MOTA	971	N	ALA A 183	18.491	31.449	22.322	1.00 15.12
ATOM	972	CA	ALA A 183	17.660	31.183	21.131	1.00 15.16
MOTA	973	С	ALA A 183	16.276	31.788	21.361	1.00 17.66
ATOM	974	ō	ALA A 183	16.053	32.526	22.377	1.00 16.26
MOTA	975	СB	ALA A 183	17.557	29.684	20.875	1.00 14.23
ATOM	976	N	TYR A 184	15.338	31.487	20.466	1.00 18.41
ATOM	977	CA	TYR A 184	13.976	32.060	20.550	1.00 17.40
MOTA	978	C	TYR A 184	12.953	31.334	21.424	1.00 18.41
ATOM	979	Õ	TYR A 184	13.131	30.135	21.807	1.00 14.95
ATOM	980	CB	TYR A 184	13.411	32.237	19.138	1.00 14.05
ATOM	981	CG	TYR A 184	14.327	33.017	18.216	1.00 10.07
MOTA	982		TYR A 184	15.295	32.367	17.446	1.00 19.30
ATOM	983		TYR A 184	14.233	34.408	18.119	1.00 19.23
ATOM	984		TYR A 184	16.144	33.083	16.599	1.00 19.03
ATOM	985		TYR A 184	15.079	35.134	17.279	1.00 19.22
ATOM	986	CEZ	TYR A 184	16.027	34.466	16.521	1.00 19.86
ATOM	987	OH	TYR A 184	16.842	35.185		1.00 19.86
ATOM	988	N	ALA A 185	11.873	32.046	21.734	1.00 20.89
AT OLI	200	1.4	WIN W TQD	11.0/2	32.040	41./34	1.00 10.29

MOTA	989	CA	ALA	Α	185	10.784	31.519	22.592	1.00 17.90
ATOM	990	С	ALA	Α	185	10.185	30.221	22.068	1.00 17.38
ATOM	991	ō	ALA			9.682	29.372	22.869	1.00 15.41
		-							
MOTA	992	CB	ALA	A	185	9.690	32.579	22.742	1.00 15.99
ATOM	993	N	GLU	Α	186	10.232	30.046	20.751	1.00 20.56
ATOM	994	CA	GLU			9.679	28.846	20.086	1.00 23.43
							27.533	20.690	1.00 23.87
MOTA	995	С	GLU			10.169			
MOTA	996	0	GLU	A	186	9.448	26.486	20.619	1.00 24.67
MOTA	997	CB	GLU	Α	186	10.009	28.887	18.591	1.00 27.60
MOTA	998	CG	GLU	Α	186	9.447	27.729	17.786	1.00 32.42
ATOM	999	CD	GLU			7.941	27.593	17.923	1.00 36.08
ATOM	1000	OE1				7.255	28.633	18.041	1.00 39.03
ATOM	1001	OE2	GLU	Α	186	7.439	26.448	17.900	1.00 37.05
ATOM	1002	N	ILE	A	187	11.363	27.540	21.283	1.00 22.31
ATOM	1003	CA	ILE	Α	187	11.904	26.302	21.900	1.00 19.35
ATOM	1004	C	ILE			12.113	26.441	23.403	1.00 20.13
ATOM	1005	0	ILE			12.887	25.654	24.034	1.00 19.35
MOTA	1006	CB	ILE	Α	187	13.241	25.872	21.248	1.00 19.03
ATOM	1007	CG1	ILE	A	187	14.270	26.998	21.355	1.00 18.36
MOTA	1008	CG2	ILE	Α	187	13.008	25.488	19.795	1.00 19.03
ATOM	1009	CD1				15.627	26.635	20.780	1.00 17.45
							•		
MOTA	1010	N	ALA			11.441	27.416	23.999	1.00 19.82
MOTA	1011	CA	ALA	A	188	11.551	27.636	25.454	1.00 20.35
ATOM	1012	C	ALA	A	188	10.622	26.661	26.171	1.00 19.60
MOTA	1013	0	ALA	Α	188	9.554	26.277	25.618	1.00 19.52
ATOM	1014	СB	ALA			11.160	29.083	25.793	1.00 17.16
								27.372	1.00 20.77
ATOM	1015	N	ARG			11.004	26.231		
ATOM	1016	CA	ARG			10.142	25.324	28.164	1.00 21.43
MOTA	1017	С	ARG	Α	189	9.577	26.162	29.303	1.00 22.80
MOTA	1018	0	ARG	Α	189	10.274	27.099	29.817	1.00 23.68
ATOM	1019	CB	ARG			10.949	24.151	28.753	1.00 22.36
								27.729	1.00 23.90
MOTA	1020	CG	ARG			11.689	23.285		
MOTA	1021	CD	ARG			10.765	22.818	26.624	1.00 24.33
MOTA	1022	NE	ARG	Α	189	11.419	21.914	25.681	1.00 25.35
ATOM	1023	CZ	ARG	A	189	11.336	20.586	25.724	1.00 27.35
MOTA	1024		ARG			10.620	19.991	26.673	1.00 24.73
ATOM	1025		ARG			11.959	19.849	24.807	1.00 25.42
MOTA	1026	N	PRO			8.325	25.890	29.725	1.00 23.27
ATOM	1027	CA	PRO	A	190	7.442	24.830	29.216	1.00 23.21
MOTA	1028	С	PRO	A	190	6.826	25.110	27.849	1.00 23.72
MOTA	1029	0	PRO	Α	190	6.458	24.157	27.101	1.00 23.77
MOTA	1030	CB	PRO			6.377	24.713	30.305	1.00 22.63
ATOM	1031	CG	PRO			6.285	26.115	30.830	1.00 24.33
MOTA	1032	CD	PRO .			7.745	26.527	30.921	1.00 22.73
MOTA	1033	N	ASP .			6.681	26.383	27.508	1.00 25.20
MOTA	1034	CA	ASP .	A	191	6.107	26.754	26.202	1.00 25.89
MOTA	1035	С	ASP .	Α	191	6.653	28.106	25.770	1.00 25.76
ATOM	1036	Ō	ASP			7.488	28.716	26.498	1.00 24.40
ATOM							26.757	26.269	1.00 28.36
	1037	CB	ASP .			4.569			
MOTA	1038	CG	ASP			4.024	27.697	27.323	1.00 30.16
MOTA	1039	OD1	ASP .	Α	191	2.887	27.468	27.783	1.00 33.88
ATOM	1040	OD2	ASP .	Α	191	4.714	28.669	27.686	1.00 30.53
MOTA	1041	N	ASP .			6.214	28.596	24.617	1.00 26.01
ATOM	1042	CA	ASP .			6.724	29.877	24.088	1.00 26.22
MOTA	1043	C	ASP .			6.236	31.123	24.813	1.00 26.52
MOTA	1044	0	ASP .	A	192	6.567	32.275	24.395	1.00 26.27
MOTA	1045	CB	ASP .	Α	192	6.419	29.985	22.589	1.00 27.69
MOTA	1046	CG	ASP .			4.940	30.161	22.296	1.00 29.61
ATOM	1047		ASP .			4.102	29.647	23.066	1.00 31.87
									1.00 30.31
MOTA	1048		ASP .			4.618	30.805	21.279	
MOTA	1049	N	SER .			5.470	30.947	25.885	1.00 24.46
MOTA	1050	CA	SER .	A	193	4.988	32.117	26.645	1.00 24.21

ATOM	1051	С	SER	Α	193	6.078	32.565	27.614	1.00 22.68
MOTA	1052	0			193	6.082	33.740	28.082	1.00 22.41
MOTA	1053	CB			193	3.701	31.787	27.415	1.00 25.67
MOTA	1054	OG	SER	Α	193	3.910	30.774	28.386	1.00 27.13
MOTA	1055	N	LEU	Α	194	7.009	31.670	27.932	1.00 20.84
ATOM	1056	CA			194	8.107	32.044	28.852	1.00 18.87
MOTA	1057	С			194	9.149	32.830	28.065	1.00 18.82
MOTA	1058	0	LEU	Α	194	10.066	32.240	27.419	1.00 19.19
MOTA	1059	CB	LEU	Ά	194	8.758	30.809	29.469	1.00 17.48
ATOM	1060	CG			194	9.680	31.201	30.631	1.00 19.18
MOTA	1061		LEU			8.825	31.633	31.825	1.00 16.80
MOTA	1062	CD2	LEU	Α	194	10.585	30.044	31.014	1.00 16.32
MOTA	1063	И	GLU	Α	195	9.025	34.150	28.095	1.00 18.44
ATOM	1064	CA			195	9.949	35.029	27.369	1.00 18.80
MOTA	1065	C			195	11.415	34.777	27.733	1.00 19.02
ATOM	1066	0	GLU	A	195	11.791	34.754	28.953	1.00 17.72
ATOM	1067	CB	GLU	Α	195	9.575	36.485	27.644	1.00 20.83
ATOM	1068	CG	GLU	Α	195	10.514	37.512	27.047	1.00 23.03
ATOM	1069	CD			195	9.989	38.926	27.204	1.00 24.10
								26.337	
MOTA	1070	OE1			195	9.211	39.373		1.00 25.77
ATOM	1071	OE2	GLU	A	195	10.343	39.585	28.203	1.00 24.06
ATOM	1072	N	PRO	A	196	12.272	34.559	26.714	1.00 18.43
MOTA	1073	CA	PRO	Α	196	13.702	34.311	26.935	1.00 18.17
ATOM	1074	C			196	14.385	35.571	27.447	1.00 16.90
ATOM	1075	0	PRO	A	196	13.845	36.715	27.297	1.00 17.67
MOTA	1076	CB	PRO	Α	196	14.210	33.914	25.546	1.00 17.79
ATOM	1077	ÇG	PRO	Α	196	12.992	33.305	24.892	1.00 19.11
ATOM	1078	CD	PRO	Ά	196	11.911	34.287	25.310	1.00 18.58
ATOM	1079	N	PHE			15.558	35.405	28.039	1.00 15.80
ATOM	1080	CA	PHE			16.290	36.550	28.574	1.00 14.47
MOTA	1081	C	PHE	A	197	16.597	37.663	27.576	1.00 16.31
MOTA	1082	0	PHE	Α	197	16.392	38.873	27.894	1.00 14.87
ATOM	1083	СВ	PHE			17.595	36.093	29.217	1.00 12.99
ATOM	1084	CG	PHE			18.472	37.227	29.652	1.00 13.09
ATOM	1085	CD1				19.376	37.806	28.767	1.00 12.33
ATOM	1086	CD2	PHE	A	197	18.347	37.766	30.926	1.00 14.29
MOTA	1087	CE1	PHE	Α	197	20.139	38.907	29.143	1.00 12.22
MOTA	1088	CE2	PHE			19.108	38.873	31.310	1.00 14.64
ATOM	1089	CZ	PHE			20.002	39.441	30.415	1.00 13.26
MOTA	1090	N	PHE			17.089	37.319	26.390	1.00 16.71
MOTA	1091	CA	PHE	Α	198	17.427	38.384	25.431	1.00 17.60
MOTA	1092	С	PHE	Α	198	16.212	39.192	25.001	1.00 17.52
MOTA	1093	0	PHE	Α	198	16.317		24.774	1.00 16.03
MOTA	1094	CB	PHE			18.133	37.829	24.196	1.00 17.77
MOTA	1095	CG	PHE			19.051	38.826	23.549	1.00 17.92
MOTA	1096	CD1	PHE	Α	198	20.310	39.075	24.087	1.00 18.66
ATOM	1097	CD2	PHE	Α	198	18.633	39.569	22.455	1.00 16.90
ATOM	1098		PHE			21.139	40.053	23.546	1.00 18.55
ATOM	1099		PHE			19.454	40.551	21.904	1.00 17.96
MOTA	1100	CZ	PHE.			20.708	40.795	22.451	1.00 18.52
MOTA	1101	N	ASP	Α	199	15.066	38.530	24.879	1.00 17.52
ATOM	1102	CA	ASP	Α	199	13.819	39.225	24.491	1.00 19.54
MOTA	1103	С	ASP			13.464	40.261	25.561	1.00 18.83
ATOM	1104	0	ASP			13.134	41.444	25.233	1.00 20.48
MOTA	1105	CB	ASP			12.685	38.210	24.338	1.00 21.95
MOTA	1106	CG	ASP	Α	199	12.868	37.312	23.126	1.00 24.77
MOTA	1107	OD1	ASP	A	199	12.408	37.687	22.028	1.00 27.27
ATOM	1108		ASP			13.481	36.234	23.261	1.00 27.11
	1109								
MOTA		N	SER			13.530	39.858	26.829	1.00 17.89
ATOM	1110	CA	SER			13.223	40.784	27.947	1.00 16.17
MOTA	1111	C	SER	Α	200	14.211	41.943	27.915	1.00 16.77
MOTA	1112	0	SER			13.823	43.140	28.072	1.00 17.20
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MOTA	1113	CB	SER	A	200		13.336	40.062	29.292	1.00	14.55
ATOM	1114	OG	SER	A	200		12.386	39.017	29.400	1.00	14.16
MOTA	1115	N	LEU	Α	201		15.481	41.617	27.711	1.00	16.47
ATOM	1116	CA			201		16.553	42.638	27.654		18.93
ATOM	1117	C			201		16.237	43.684	26.586		18.88
ATOM	1118	Ö			201		16.274		26.852		18.26
ATOM	1119	CB			201		17.884		27.337		18.68
ATOM	1120	CG			201		19.244		27.523		20.59
ATOM	1121	-	LEU					42.616	26.194		20.98
ATOM	1122	CD2			201		19.100	44.053	28.045		20.13
MOTA	1123	Ŋ			202		15.919	43.222	25.383		20.38
ATOM	1124	CA			202		15.600	44.130	24.264		20.23
MOTA	1125	С			202		14.335	44.938	24.532		23.13
MOTA	1126	0			202		14.284	46.175	24.255		23.36
MOTA	1127	CB			202		15.433	43.337	22.948		19.84
MOTA	1128		VAL				14.830	44.228	21.855	1.00	
MOTA	1129		VAL				16.792	42.804	22.502	1.00	
MOTA	1130	N			203		13.315	44.285	25.074	1.00	24.15
ATOM	1131	CA	LYS	Α	203		12.050	44.985	25.360	1.00	27.77
ATOM	1132	C			203	•	12.178	46.049	26.452		27.47
MOTA	1133	0	LYS	Α	203		11.753	47.223	26.252	1.00	26.63
MOTA	1134	CB	LYS	Α	203		10.970	43.973	25.746	1.00	29.55
ATOM	1135	CG	LYS	Α	203		9.609	44.594	26.008	1.00	34.08
ATOM	1136	CD	LYS	Α	203		8.497	43.798	25.335	1.00	36.82
MOTA	1137	CE	LYS	Α	203		8.504	42.342	25.774	1.00	38.97
ATOM	1138	NZ	LYS	Α	203		7.512	41.533	25.012	1.00	40.86
ATOM	1139	N	GLN	Α	204		12.771	45.687	27.585	1.00	26.46
ATOM	1140	CA	GLN	Α	204		12.910	46.632	28.721	1.00	26.94
ATOM	1141	C	GLN	Α	204		14.125	47.542	28.614		28.51
ATOM	1142	0			204		14.479	48.264	29.600		30.36
ATOM	1143	CB	GLN				13.007	45.848	30.032		24.17
ATOM	1144	CG	GLN				11.980	44.739	30.170		20.78
ATOM	1145	CD	GLN			,	12.270	43.821	31.342		20.14
ATOM	1146		GLN			·	11.725	42.676	31.420		19.72
ATOM	1147	NE2					13.107	44.279	32.265		16.56
ATOM	1148	N	THR				14.762	47.568	27.453		28.58
ATOM	1149	CA	THR				15.979	48.375	27.306		29.06
ATOM	1150	C	THR				16.186	48.905	25.885		30.58
ATOM	1151	Ö	THR				15.427	48.525	24.940		30.23
ATOM	1152	СВ	THR				17.175	47.501	27.772		29.85
ATOM	1153		THR				17.572	47.899	29.088		29.62
-ATOM	1154	CG2					18.328	47.576	26.823		29.02
ATOM	1155	N N	HIS				17.175	49.784	25.711		31.92
ATOM	1156	CA	HIS				17.488	50.350	24.372	1.00	
ATOM	1157	C	HIS				18.548	49.530	23.637	1.00	
ATOM	1158	0	HIS				18.905	49.845	22.460	1.00	
ATOM	1159	СВ	HIS				17.975		24.487	1.00	
ATOM	1160	CG	HIS					51.799		1.00	
							16.898	52.773	24.848		
ATOM ATOM	1161		HIS HIS			•	15.696	52.836	24.177	1.00	
	1162						16.849	53.736	25.800	1.00	
ATOM	1163		HIS				14.951	53.794	24.699	1.00	
ATOM	1164		HIS				15.627	54.356	25.685	1.00	
ATOM	1165	N	VAL				19.075	48.501	24.291	1.00	
ATOM	1166	CA	VAL				20.097	47.639	23.651	1.00	
ATOM	1167	С	VAL				19.511	47.083	22.354	1.00	
MOTA	1168	0	VAL				18.415	46.441	22.358	1.00	
MOTA	1169	CB	VAL				20.498	46.462	24.572	1.00	
MOTA	1170		VAL				21.399	45.491	23.825	1.00	
MOTA	1171		VAL				21.219	46.987	25.805	1.00	
MOTA	1172	N	PRO				20.192	47.311	21.220	1.00	
MOTA	1173	CA	PRO				19.683	46.804	19.944	1.00	
MOTA	1174	С	PRO	A	208		19.547	45.284	19.914	1.00	22.81

MOTA	1175	0	PRO	A	208	20.290	44.545	20.630	1.00	21.12
MOTA	1176	CB	PRO	A	208	20.689	47.343	18.926		24.65
MOTA	1177	CG	PRO	Α	208	21.927	47.510	19.711	1.00	25.77
MOTA	1178	CD	PRO	A	208	21.441	48.062	21.025	1.00	24.39
ATOM	1179	N	ASN	A	209	18.605	44.806	19.109	1.00	21.59
MOTA	1180	CA	ASN	Α	209	18.322	43.362	18.995	1.00	20.43
MOTA	1181	С	ASN	Α	209	19.390	42.599	18.222	1.00	20.52
MOTA	1182	0	ASN	Α	209	19.190	42.217	17.026	1.00	21.39
MOTA	1183	CB	ASN	Α	209	16.957	43.159	18.340	1.00	18.52
ATOM	1184	CG	ASN	A	209	16.501	41.728	18.402	1.00	18.12
MOTA	1185	OD1	ASN	A	209	16.968	40.948	19.281		18.32
MOTA	1186	ND2	ASN	A	209	15.594	41.348	17.513	1.00	15.63
MOTA	1187	N	LEU	Α	210	20.514	42.346	18.883	1.00	19.53
ATOM	1188	CA	LEU	Α	210	21.631	41.634	18.243	1.00	19.83
ATOM	1189	C	LEU	A	210	22.765	41.421	19.226	1.00	19.02
ATOM	1190	0	LEU	A	210	22.958	42.238	20.176	1.00	18.52
ATOM	1191	CB	LEU	A	210	22.120	42.451	17.035	1.00	21.93
MOTA	1192	CG	LEU	Α	210	23.534	42.305	16.456		22.75
MOTA	1193		LEU			23.612	43.009	15.102		23.20
MOTA	1194	CD2	LEU			24.548	42.910	17.409		24.60
ATOM	1195	N	PHE	A	211	23.509	40.334	19.044		16.48
ATOM	1196	CA	PHE	Α	211	24.671	40.055	19.909	1.00	16.70
MOTA	1197	С	PHE			25.722	39.310	19.095		16.08
MOTA	1198	0	PHE			25.392	38.653	18.063		17.22
MOTA	1199	CB	PHE			24.251	39.280	21.173		14.67
ATOM	1200	CG	PHE			23.813	37.863	20.924		16.01
ATOM	1201		PHE			24.748	36.837	20.835		14.91
MOTA	1202		PHE			22.465	37.546	20.824	1.00	
MOTA	1203		PHE			24.344	35.515	20.653	1.00	
MOTA	1204	CE2	PHE			22.054	36.224	20.641	1.00	
MOTA	1205	CZ	PHE			22.996	35.207	20.558	1.00	
MOTA	1206	N	SER			26.977	39.424	19.520	1.00	
ATOM	1207	CA	SER			28.126	38.803	18.818	1.00	
MOTA	1208	C	SER			28.894	37.862	19.725	1.00	
ATOM	1209	0	SER			29.036	38.122	20.955	1.00	
MOTA	1210	CB	SER			29.094	39.888	18.349	1.00	
MOTA	1211	OG	SER			28.431	40.869	17.593	1.00	
MOTA	1212	N	LEU			29.430	36.797 35.819	19.144 19.930	1.00	
MOTA	1213 1214	CA C	LEU			30.194			1.00	
MOTA MOTA	1214	0	LEU			31.563 31.702	35.509 35.162	19.352 18.137	1.00	
ATOM	1216	СВ	LEU			29.394	34.522	20.060	1.00	
ATOM	1217	CG	LEU			28.735	34.322	21.408	1.00	
ATOM	1218		LEU			28.196	35.475	22.050	1.00	
MOTA	1219		LEU			27.627	33.185	21.192	1.00	
ATOM	1220	N	GLN .			32.581	35.656	20.191	1.00	
MOTA	1221	CA	GLN			33.954	35.324	19.797	1.00	
ATOM	1222	C	GLN			34.407	34.258	20.778	1.00	
MOTA	1223		GLN .			34.848	34.582	21.917	1.00	
MOTA	1224		GLN .			34.903	36.523	19.914	1.00	
MOTA	1225	CG	GLN .			36.290	36.231	19.341	1.00	
ATOM	1226	CD	GLN .			37.397	37.099	19.932	1.00	
ATOM	1227					38.459	37.332	19.273	1.00 2	
MOTA			GLN			37.199	37.571	21.156	1.00 2	
ATOM	1229	N	LEU :			34.284	32.997	20.390	1.00	
MOTA	1230		LEU .			34.729	31.890.		1.00	
MOTA	1231		LEU Z			36.193	31.625	20.925	1.00	
MOTA	1232		LEU			36.541	31.357	19.737	1.00 1	
MOTA	1233	СВ	LEU 2	<b>A</b> :	215	33.872	30.644	21.005	1.00 1	
MOTA		CG	LEU 2	A :	215	32.636	30.429	21.893	1.00 1	
MOTA			LEU 2			31.900	31.734	22.143	1.00 1	13.31
MOTA	1236	CD2	LEU 2	A :	215	31.723	29.407	21.240	1.00 1	

MOTA	1237	N	CYS A	216	37.066	31.706	21.922	1.00 14.83
MOTA	1238	CA	CYS A	216	38.504	31.486	21.682	1.00 16.37
MOTA	1239	С	CYS A	216 .	39.066	30.196	22.263	1.00 17.20
MOTA	1240	0	CYS A	216	39.174	30.046	23.519	1.00 16.79
MOTA	1241	CB	CYS A		39.314	32.668	22.227	1.00 19.03
MOTA	1242	SG	CYS A		38.852	34.278	21.505	1.00 23.75
ATOM	1243	N	GLY A		39.415	29.257	21.387	1.00 15.43
ATOM	1244	CA	GLY A		40.018	28.021	21.843	1.00 16.40
ATOM	1245	C	GLY A		41.483	28.371	22.064	1.00 17.87
ATOM	1246	Ö	GLY A		42.057	29.204	21.303	1.00 17.53
ATOM	1247	N	ALA A		42.119	27.785	23.069	1.00 17.33
MOTA	1247	CA	ALA A		43.539	28.108	23.349	1.00 17.73
		CA	ALA A		44.486	27.408	22.379	1.00 10.33
ATOM	1249							
ATOM	1250	0	ALA A		45.602	27.927	22.069	1.00 16.46
ATOM	1251	CB	ALA A		43.884	27.731	24.779	1.00 14.95
ATOM	1252	N	GLY A		44.073	26.245	21.890	1.00 16.19
ATOM	1253	CA	GLY A		44.909	25.505	20.970	1.00 17.57
ATOM	1254	C	GLY A		45.696	24.439	21.703	1.00 17.52
MOTA	1255	0	GLY A		46.490	23.675	21.076	1.00 16.29
ATOM	1256	N	PHE A		45.502	24.375	23.018	1.00 17.13
MOTA	1257	CA	PHE A		46.190	23.381	23.873	1.00 18.29
ATOM	1258	C	PHE A		45.381	23.185	25.153	1.00 19.24
MOTA	1259	0	PHE A		44.477	24.012	25.475	1.00 19.69
MOTA	1260	CB	PHE A		47.616	23.854	24.187	1.00 18.72
MOTA	1261	CG	PHE A		47.689	25.253	24.731	1.00 20.07
MOTA	1262		PHE A		47.448	25.507	26.077	1.00 20.91
MOTA	1263	CD2	PHE A	220	47.984	26.320	23.890	1.00 19.91
MOTA	1264	CE1	PHE A	220	47.505	26.809	26.576	1.00 21.79
MOTA	1265	CE2	PHE A	220	48.043	27.620	24.374	1.00 20.35
MOTA	1266	CZ	PHE A	220	47.802	27.866	25.721	1.00 21.77
ATOM	1267	N	PRO A	221	45.65 <i>9</i>	22.110	25.907	1.00 20.17
MOTA	1268	CA	PRO A	221	44.922	21.846	27.147	1.00 21.27
MOTA	1269	С	PRO A	221	45.014	22.959	28.180	1.00 23.04
MOTA	1270	0	PRO A	221	46.065	23.666	28.292	1.00 23.99
MOTA	1271	CB	PRO A	221	45.545	20.543	27.648	1.00 20.22
ATOM	1272	CG	PRO A	221	45.946	19.855	26.390	1.00 20.63
MOTA	1273	CD	PRO A	221	46.571	20.994	25.602	1.00 20.45
MOTA	1274	N	LEU A	222	43.934	23.132	28.933	1.00 25.72
MOTA	1275	CA	LEU A	222	43.873	24.158	29.991	1.00 28.32
MOTA	1276	С	LEU A	222	43.425	23,516	31.291	1.00 30.88
ATOM	1277	0	LEU A	222	42.248	23.042	31.403	1.00 31.71
ATOM	1278	CB	LEU A	222 -	42.880	25.261	29.620	1.00 27.52
ATOM	1279	CG				26.233	28.506	
ATOM	1280		LEU A			27.042	28.096	1.00 26.79
ATOM	1281		LEU A		44.382	27.143	28.983	1.00 27.13
MOTA	1282	N	ASN A		44.320	23.470	32.273	1.00 34.15
MOTA	1283	CA	ASN A	223	43.959	22.893	33.583	1.00 37.64
MOTA	1284	С	ASN A		43.014	23.882	34.254	1.00 38.54
ATOM	1285	Ō	ASN A		42.864	25.056	33.785	1.00 36.72
ATOM	1286	CB	ASN A			22.663	34.457	1.00 38.54
MOTA	1287	CG	ASN A			23.952	34.839	1.00 39.09
ATOM	1288		ASN A			24.903	35.375	1.00 41.39
ATOM	1289		ASN A			24.013	34.595	1.00 40.09
ATOM	1290	N	GLN A			23.444	35.335	1.00 41.79
MOTA	1291	CA	GLN A			24.278	36.073	1.00 41.79
ATOM	1292	C	GLN A			25.708	36.359	1.00 42.52
MOTA	1293	0	GLN A		41.138	26.705	36.126	1.00 42.75
MOTA	1294	CB	GLN A		41.138	23.572	37.378	1.00 42.75
MOTA	1295	CG	GLN A			23.956	37.376	1.00 49.86
ATOM	1296	CD	GLN A			23.160	38.990	1.00 49.88
ATOM	1297		GLN A			23.100	39.443	1.00 51.40
ATOM	1298		GLN A		39.866		39.496	1.00 52.42
TION	- L J Q	1447	JAN A	- 4 T	39.000	24.413	JJ. 730	±.00 J4./J

MOTA	1299	N	SER	Α	225	43.133	25.852	36.831	1.00 40.27
MOTA	1300	CA	SER	Α	225	43.669	27.200	37.138	1.00 39.30
ATOM	1301	С			225	43.989	28.028	35.893	1.00 36.57
ATOM	1302	Ó	SER	Α	225	43.920	29.292	35.930	1.00 36.27
MOTA	1303	СВ			225	44.917	27.094	38.027	1.00 40.27
ATOM	1304	OG			225	45.974	26.411	37.376	1.00 42.21
ATOM	1305	N			226	44.339	27.364	34.796	1.00 34.29
ATOM	1306	CA			226	44.654	28.083	33.542	1.00 32.79
ATOM	1307	C			226	43.375	28.651	32.954	1.00 31.17
ATOM	1308	0			226	43.354	29.815	32.454	1.00 29.09
ATOM	1309	CB			226	45.307	27.144	32.526	1.00 33.69
ATOM	1310	CG			226	46.708	26.696	32.902	1.00 36.40
ATOM	1311	CD			226	47.251	25.619	31.972	1.00 37.70
ATOM	1312		GLU			46.585	24.567	31.830	1.00 37.70
ATOM	1312	OE2			226	48.340	25.823	31.389	1.00 37.14
					227	42.305	27.867	33.007	1.00 37.14
MOTA	1314	N CA			227	41.013	28.312	32.458	1.00 29.89
MOTA	1315					40.512	29.547	33.203	1.00 30.15
ATOM	1316	C			227				
ATOM	1317	0			227	39.922	30.484	32.582	1.00 30.30
MOTA	1318	CB			227	39.940	27.210	32.558	1.00 30.93
ATOM	1319		VAL			38.800	27.538	31.637	1.00 32.67
ATOM	1320		VAL			40.516	25.867	32.183	1.00 32.31
MOTA	1321	N	LEU			40.731	29.581	34.513	1.00 28.88
MOTA	1322	CA.			228	40.292	30.726	35.336	1.00 27.31
ATOM	1323	C	LEU			41.059	31.992	34.975	1.00 27.59
MOTA	1324	0	LEU			40.491	33.129	35.020	1.00 27.84
ATOM	1325	CB	LEU			40.496	30.420	36.819	1.00 27.50
MOTA	1326	CG	LEU			39.700	29.259	37.419	1.00 29.32
MOTA	1327		LEU			40.129	29.053	38.867	1.00 28.16
MOTA	1328		LEU			38.205	29.549	37.339	1.00 28.58
ATOM	1329	N	ALA			42.327	31.835	34.610	1.00 27.12
MOTA	1330	CA	ALA			43.176	32.998	34.257	1.00 27.64
ATOM	1331	С	ALA			43.134	33.347	32.776	1.00 27.65
ATOM	1332	0	ALA			43.460	34.504	32.375	1.00 29.94
ATOM	1333	CB	ALA			44.617		34.682	1.00 27.52
MOTA	1334	N	SER			42.736	32.393	31.947	1.00 26.68
ATOM	1335	CA	SER			42.692	32.635	30.498	1.00 26.33
MOTA	1336	C	SER			41.438	33.360	30.032	1.00 26.22
MOTA	1337	0	SER			40.356	33.302	30.695	1.00 25.70
MOTA	1338	CB	SER			42.815	31.310	29.746	1.00 26.07
MOTA	1339	OG	SER			42.759	31,519	28.344	1.00 26.54
ATOM	1340	И.	VAL			41.562	34.056	28.909	1.00 25.03
MOTA	1341	CA	VAL			40.415		28.320	1.00 24.89
ATOM	1342	C	VAL			39.785	33.776		1.00 24.75
ATOM	1343	0	VAL			40.453	33.310	26.371	1.00 25.97
MOTA	1344	CB	VAL			40.859	36.043	27.568	1.00 24.38
MOTA	1345		VAL			39.729	36.554	26.678	1.00 22.98
MOTA	1346		VAL			41.244	37.119	28.577	1.00 23.20
MOTA	1347	N	GLY			38.526	33.433	27.588	1.00 23.26
MOTA	1348	CA	GLY			37.846	32.481	26.729	1.00 22.77
MOTA	1349	C	GLY			37.125	33.081	25.538	1.00 21.57
MOTA	1350	0	GLY			36.590	32.324	24.666	1.00 20.69
MOTA	1351	N	GLY			37.078	34.408	25.468	1.00 19.21
MOTA	1352	CA	GLY			36.410	35.050	24.353	1.00 17.96
ATOM	1353	C	GLY			35.599	36.275	24.731	1.00 18.25
MOTA	1354	0	GLY			35.778	36.866	25.851	1.00 15.19
MOTA	1355	N	SER			34.708	36.677	23.828	1.00 16.58
MOTA	1356	CA	SER			33.864	37.864	24.053	1.00 16.83
MOTA	1357	C	SER			32.423	37.667	23.599	1.00 17.82
ATOM	1358	0	SER				36.995	22.552	1.00 17.90
MOTA	1359	CB	SER				39.072	23.291	1.00 16.36
MOTA	1360	OG	SER	Α	234	35.816	39.253	23.508	1.00 18.23
						20/55			

ATOM	1361	N	MET .	Α	235	31.506	38.227	24.372	1.00	18.00
ATOM	1362	CA	MET .	Α	235	30.091	38.201	24.010	1.00	17.58
ATOM	1363	C	MET			29.732	39.677	23.996	1.00	18.27
	1364	Ö	MET			29.594	40.322	25.087		19.03
MOTA										
ATOM	1365	CB	MET .			29.232	37.475	25.046		16.91
MOTA	1366	CG	MET .	Α	235	27.759	37.455	24.634		17.60
MOTA	1367	SD	MET .	Α	235	26.597	36.751	25.819	1.00	20.56
ATOM	1368	CE	MET .	A	235	25.105	36.803	24.857	1.00	21.69
ATOM	1369	N	ILE .			29.629	40.248	22.801	1.00	19.70
ATOM	1370	CA	ILE .			29.271	41.669	22.674		19.40
								22.522		20.06
ATOM	1371	C	ILE .			27.764	41.758			
ATOM	1372	0	ILE .			27.175	41.365	21.467		16.87
ATOM	1373	СВ	ILE .			29.985	42.341	21.470		21.41
MOTA	1374	CG1	ILE .	Α	236	31.452	42.625	21.821	1.00	22.57
MOTA	1375	CG2	ILE .	Α	236	29.329	43.672	21.149	1.00	21.72
MOTA	1376	CD1	ILE .	Α	236	32.243	41.426	22.228	1.00	25.65
ATOM	1377	N	ILE .	Α	237	27.122	42.246	23.575	1.00	20.16
ATOM	1378	CA	ILE .			25.663	42.382	23.599		21.01
			ILE .			25.215	43.710	22.996		22.16
ATOM	1379	C								
MOTA	1380	0	ILE .			25.620	44.812	23.472		22.96
MOTA	1381	CB	ILE .			25.153	42.241	25.050		21.36
MOTA	1382	CG1	ILE .	A	237	25.346	40.791	25.498	1.00	22.29
MOTA	1383	CG2	ILE .	A	237	23.694	42.660	25.156	1.00	20.45
ATOM	1384	CD1	ILE :	A	237	25.002	40.529	26.939	1.00	24.84
ATOM	1385	N	GLY 2			24.404	43.626	21.946	1.00	23.30
ATOM	1386	CA	GLY 2			23.903	44.820	21.288		25.11
ATOM	1387	C	GLY A			24.821	45.437	20.244		26.35
MOTA	1388	0	GLY 2			24.644	46.640	19.874		27.08
MOTA	1389	N	GLY 2			25.792	44.681	19.743		25.50
MOTA	1390	CA	GLY 2	A	239	26.679	45.251	18.747		24.81
ATOM	1391	C	GLY A	A	239	27.807	44.371	18.242	1.00	26.38
MOTA	1392	0	GLY :	A	239	27.942	43.167	18.632	1.00	23.61
ATOM	1393	N	ILE :			28.632	44.960	17.383	1.00	26.33
ATOM	1394	CA	ILE 2			29.780	44.273	16.758		25.87
ATOM	1395	C	ILE A			31.067	45.033	17.055		26.95
						31.121	46.287	16.882		28.86
ATOM	1396	0	ILE A							
ATOM	1397	CB	ILE A			29.607	44.226	15.226		25.88
MOTA	1398	CG1	ILE A			28.298	43.519	14.871		25.12
MOTA	1399	CG2	ILE A	A	240	30.806	43.541	14.581	1.00	26.56
MOTA	1400	CD1	ILE A	A	240	27.939	43.599	13.396	1.00	24.59
MOTA	1401	N	ASP 2	Α	241	32.100	44.323	17.498	1.00	25.24
MOTA	1402	CA	ASP 2	A	241	33.395	44.973	17.781	1.00	25.13
MOTA	1403	С	ASP Z	Α	241	34.383	44.548	16.698	1.00	26.31
ATOM	1404	Ō	ASP Z				43.326	16.536	1.00	
ATOM	1405	СВ	ASP A				44.561	19.153	1.00	
			ASP A				45.325	19.541		
ATOM	1406	CG							1.00	
MOTA	1407		ASP A			35.144	46.032	20.567	1.00	
MOTA	1408		ASP A			36.180	45.226	18.817	1.00	
MOTA	1409	N	HIS A			34.913	45.517	15.960	1.00	26.86
MOTA	1410	CA	HIS A	Α	242	35.853	45.222	14.852	1.00	27.45
MOTA	1411	С	HIS A	A	242	37.197	44.613	15.221	1.00	25.41
ATOM	1412	0	HIS A	A	242	37.871	43.998	14.347	1.00	23.94
ATOM	1413	СВ	HIS 2			36.085	46.481	14.013	1.00	
ATOM	1414	CG	HIS 2			34.858	46.957	13.304	1.00	
ATOM	1415		HIS A			33.822	47.591	13.956	1.00	
MOTA	1416		HIS A				46.837		1.00	
MOTA	1417		HIS A				47.840		1.00	
MOTA	1418	NE2	HIS A				47.392		1.00	40.36
MOTA	1419	N	SER A	Ą	243	37.615	44.751	16.471	1.00	22.23
MOTA	1420	CA	SER A	Ą	243		44.184		1.00	22.06
ATOM	1421	C	SER A			38.843			1.00	
ATOM	1422	Ō	SER A			39.897		17.130	1.00	
		-		-		22.031	,			

ATOM	1423	СВ	SER A	243	39.368	44.785	18.211	1.00	22.47
MOTA	1424	OG	SER A		38.515	44.386	19.274	1.00	23.32
ATOM	1425	N	LEU A		37.635	42.115	16.979		20.52
ATOM	1426	CA	LEU A		37.454	40.649	17.145		18.32
ATOM	1427	C	LEU A		37.535	39.844	15.860		18.66
MOTA	1428	Ö	LEU A		37.482	38.576	15.892		18.25
	1429				36.120	40.368	17.843		18.01
MOTA		CB	LEU A						
MOTA	1430	CG	LEU A		35.998	41.054	19.206		17.93
MOTA	1431	CD1	LEU A		34.689	40.666	19.885		17.04
ATOM	1432	CD2	LEU A		37.189	40.661	20.063		19.23
MOTA	1433	N	TYR A		37.666	40.522	14.729		18.73
ATOM	1434	CA	TYR A		37.756	39.795	13.459		19.72
MOTA	1435	С	TYR A		38.536	40.545	12.398		20.55
MOTA	1436	0	TYR A		38.819	41.771	12.542		21.10
MOTA	1437	CB	TYR A		36.357	39.494	12.924		19.56
ATOM	1438	CG	TYR A	245	35.606	40.708	12.421		20.40
ATOM	1439	CD1	TYR A	245	34.977	41.586	13.302		20.11
MOTA	1440	CD2	TYR A	245	35.512	40.966	11.055		20.70
MOTA	1441	CE1	TYR A	245	34.265	42.689	12.834	1.00	21.90
MOTA	1442	CE2	TYR A	245	34.809	42.060	10.573	1.00	22.10
ATOM	1443	ĊZ	TYR A	245	34.184	42.919	11.466	1.00	23.05
ATOM	1444	ÓН	TYR A	245	33.476	43.993	10.979	1.00	22.53
ATOM	1445	N	THR A	246	38.902	39.829	11.340	1.00	20.48
MOTA	1446	CA	THR A	246	39.621	40.429	10.195	1.00	19.46
ATOM	1447	С	THR A	246	38.811	40.054	8.964	1.00	19.29
ATOM	1448	Ō	THR A		37.999	39.085	9.000	1.00	16.84
ATOM	-	CB	THR A		41.049	39.865	10.031	1.00	19.69
ATOM	1450	OG1	THR A		40.997	38.434	9.953		20.05
ATOM	1451	CG2	THR A		41.929	40.294	11.194	1.00	19.01
ATOM	1452	N	GLY A		38.996	40.793	7.879		19.48
ATOM	1453	CA	GLY A		38.259	40.490	6.668		19.61
MOTA	1454	C	GLY A		36.812	40.927	6.747		20.26
MOTA	1455	0	GLY A		36.412	41.712	7.660		21.64
ATOM	1456	N	SER A		36.006	40.437	5.816		21.23
MOTA	1457	CA	SER A		34.580	40.806	5.765		23.54
ATOM	1458	C	SER A		33.649	39.836	6.484		23.00
ATOM	1459	0	SER A		33.978	38.625	6.684		21.96
ATOM	1460	CB	SER A		34.135	40.936	4.304		24.06
MOTA	1461	OG	SER A		34.814	41.999	3.656		28.27
ATOM	1462	N	LEU A		32.494	40.355	6.881	1.00	
MOTA	1463	CA	LEU A		31.453	39.551	7.550		23.71
	1464	C	LEU A		30.478	39.103	6.468		23.26
ATOM	1465	0	LEU A		29.913	39.958	5.721		24.66
ATOM	1466	CB	LEU A		30.687	40.392	8.576		22.83
MOTA MOTA	1467	CG	LEU A		31.234	40.585	9.992		23.68
	1468		LEU A		30.483	41.728	10.659		23.07
MOTA					31.077	39.299	10.802		22.16
ATOM	1469		LEU A			37.797	6.335		21.28
MOTA	1470	N	TRP A		30.285	37.282	5.348		18.03
MOTA	1471	CA			29.328		6.115		18.51
MOTA	1472	C	TRP A		28.115	36.810	7.153		18.65
MOTA	1473	0	TRP A		28.242	36.079			19.15
MOTA	1474	CB	TRP A		29.925	36.128	4.550		
MOTA	1475	CG	TRP A		30.759	36.597	3.411		19.10 18.51
ATOM	1476	CD1			32.061	36.998	3.456		
ATOM	1477	CD2			30.328	36.777	2.058		18.74
ATOM	1478	NE1	TRP A		32.470	37.418	2.214		18.41
ATOM	1479	CE2	TRP A		31.425	37.294	1.336		18.71
MOTA	1480	CE3			29.118	36.554	1.386		19.61
MOTA	1481	CZ2			31.352	37.594	-0.029		18.57
MOTA	1482	CZ3	TRP A		29.043	36.853	0.026		20.92
MOTA	1483	CH2	TRP A		30.158	37.369	-0.666		17.98
MOTA	1484	N	TYR A	251 ·	26.939	37.203	5.644	1.00	17.22

MOTA	1485	CA			251	25.699	36.825	6.328	1.00	16.85
MOTA	1486	С	TYR	A	251	24.875	35.751	5.642		16.82
MOTA	1487.	. 0	TYR	A	251	24.668	35.782	4.397		17.05
ATOM	1488	CB	TYR	A	251	24.814	38.059	6.536		17.46
ATOM	1489	CG	TYR	A	251	25.389	39.070	7.493		17.27
ATOM	1490	CD1	TYR	Α	251	26.265	40.065	7.055		18.34
MOTA	1491	CD2	TYR	Α	251	25.076	39.018	8.852		16.39
MOTA	1492	CE1			251	26.819	40.984	7.955		18.20
ATOM	1493	CE2			251	25.622	39.925	9.753		17.81
MOTA	1494	CZ			251	26.487	40.900	9.302		17.43
MOTA	1495	OH	TYR	A	251	27.014	41.779	10.215		20.25
ATOM	1496	N			252	24.395	34.803	6.436		15.07
ATOM	1497	CA			252	23.525	33.725	5.933		14.48
MOTA	1498	C	THR			22.204	33.996	6.646		16.15
ATOM	1499	0			252	22.193	34.429	7.845		16.66
ATOM	1500	CB	THR	Α	252	24.056	32.325	6.330		14.69
ATOM	1501	OG1				23.273	31.316	5.684		13.97
MOTA	1502	CG2	THR	Α	252	23.974	32.118	7.839		14.05
MOTA	1503	N	PRO	Α	253	21.070	33.774	5.972		15.93
MOTA	1504	CA	PRO	Α	253	19.826	34.054	6.694		17.09
ATOM	1505	C	PRO	A	253	19.418	33.029	7.741	1.00	18.67
MOTA	1506	0	PRO	Α	253	19.782	31.813	7.653	1.00	17.11
MOTA	1507	CB	PRO	Α	253	18.789	34.161	5.572	1.00	17.20
MOTA	1508	CG	PRO	A	253	19.304	33.207	4.545	1.00	17.18
MOTA	1509	CD	PRO			20.809	33.468	4.553	1.00	17.14
MOTA	1510	N	ILE			18.692	33.501	8.750	1.00	18.82
MOTA	1511	CA	ILE			18.165	32.604	9.792	1.00	20.14
MOTA	1512	C	ILE			16.885	32.091	9.137	1.00	21.33
MOTA	1513	0	ILE			15.911	32.875	8.914	1.00	21.52
MOTA	1514	CB	ILE			17.827	33.368	11.091	1.00	20.62
MOTA	1515	CG1				19.124	33.752	11.806		20.82
MOTA	1516	CG2				16.935	32.509	11.994	1.00	19.41
MOTA	1517	CD1				18.920	34.458	13.127		22.19
ATOM	1518	N	ARG			16.868	30.810	8.795		22.06
ATOM	1519	CA	ARG			15.702	30.211	8.115		23.47
MOTA	1520	С	ARG			14.398	30.343	8.880		24.68
MOTA	1521	0	ARG			13.334	30.719	8.299		25.49
MOTA	1522 1523	CB	ARG			15.951	28.735	7.852		22.62
MOTA		CG	ARG			14.843	28.093	7.053		22.10
ATOM ATOM	1524 1525	CD NE	ARG ARG			14.985	26.598	7.069		22.76
MOTA	1526	CZ	ARG			14.031	25.958 24.679	6.176		22.51
MOTA	1527	NH1				13.692 14.232	23.914	6.256 7.195	1.00	22.37
ATOM	1528		ARG			12.819	24.166	5.396	1.00	
	1529	N	ARG			14.451	30.023	10.165	1.00	
ATOM	1530	CA	ARG			13.264	30.085	11.029	1.00	
MOTA	1531	C	ARG			13.723	30.441	12.438	1.00	
ATOM	1532	ō	ARG			14.829	30.013	12.893	1.00	
ATOM	1533	СВ	ARG			12.561	28.729	11.009	1.00	
MOTA	1534	CG	ARG			11.350	28.599	11.914	1.00	
MOTA	1535	CD	ARG			10.878	27.150	11.899	1.00	
ATOM	1536	NE	ARG			10.180	26.788	13.126	1.00	
ATOM	1537	ĊZ	ARG			10.043	25.543	13.563	1.00	
ATOM	1538		ARG			10.559	24.535	12.870	1.00	
ATOM	1539		ARG			9.398	25.307	14.698	1.00	
MOTA	1540	N	GLU			12.914	31.219	13.141	1.00	
ATOM	1541	CA	GLU			13.270	31.650	14.500	1.00	
ATOM	1542	С	GLU			12.829	30.739	15.636	1.00	
ATOM	1543	0	GLU			11.749	30.947	16.264	1.00	
ATOM	1544	СВ	GLU			12.739	33.055	14.748	1.00	
MOTA	1545	CG	GLU	<b>A</b> :	257	13.439	34.123	13.930	1.00	
ATOM	1546	CD	GLU	A :	257	12.572	35.353	13.746	1.00	

MOTA	1547	OE1	GLU A	. 25	7	13.124	36.470	13.673	1.00	27.35
ATOM	1548	OE2	GLU A	25	7 ·	11.334	35.197	13.665	1.00	30.46
ATOM	1549	N	TRP A			13.632	29.719	15.898	1.00	19.64
ATOM	1550	CA	TRP F			13.390	28.798	17.016		19.75
			TRP I			14.812	28.548	17.495		19.46
ATOM	1551	C								
MOTA	1552	0	TRP A			15.267	29.190	18.500		20.47
ATOM	1553	CB	TRP A			12.632	27.537	16.561		18.27
MOTA	1554	CG	TRP A	25	8	13.203	26.710	15.455	1.00	17.96
ATOM	1555	CD1	TRP A	25	8	13.898	27.143	14.364	1.00	18.43
ATOM	1556	CD2	TRP A	25	8	13.051	25.293	15.298	1.00	17.87
ATOM	1557		TRP F			14.187	26.082	13.537	1.00	18.62
ATOM	1558	CE2	TRP F			13.678	24.935	14.088		17.86
						12.441	24.291	16.067		17.50
ATOM	1559.	CE3	TRP A				23.614			19.19
ATOM	1560	CZ2	TRP A			13.717		13.624		
ATOM	1561	CZ3	TRP F			12.477	22.976	15.608		19.16
ATOM	1562	CH2	TRP A			13.113	22.650	14.396		18.86
ATOM	1563	N	TYR A	25	9	15.538	27.670	16.814		18.33
ATOM	1564	CA	TYR A	25	9	16.965	27.458	17.126		15.42
ATOM	1565	С	TYR A	25	9	17.550	28.474	16.157	1.00	16.46
ATOM	1566	0	TYR A	. 25	9	16.789	29.066	15.323	1.00	15.71
ATOM	1567	CB	TYR A	25	9	17.439	26.078	16.671	1.00	13.86
ATOM	1568	CG	TYR A			17.056	24.927	17.564	1.00	13.98
ATOM	1569	CD1	TYR A			17.876	24.539	18.627		13.32
						15.875	24.224	17.346		12.14
MOTA	1570	CD2	TYR A							15.06
ATOM	1571	CE1	TYR F			17.520	23.467	19.450		
ATOM	1572	CE2	TYR A			15.510	23.167	18.155		14.24
ATOM	1573	CZ	TYR A			16.329	22.789	19.200		14.26
MOTA	1574	OH	TYR A	. 25	9	15.940	21.719	19.955		12.92
MOTA	1575	N	TYR A	. 26	0	18.851	28.725	16.224	1.00	14.50
ATOM	1576	CA	TYR A	26	0	19.440	29.630	15.232	1.00	15.21
ATOM	1577	С	TYR A	26	0	19.716	28.718	14.037	1.00	15.90
ATOM	1578	0	TYR A	26	0	20.866	28.210	13.836	1.00	16.76
ATOM	1579	СВ	TYR A			20.722	30.269	15.759	1.00	13.84
ATOM	1580	CG	TYR A			20.426	31.416	16.690	1.00	14.32
ATOM	1581	CD1	TYR A			20.534	31.270	18.078	1.00	13.41
ATOM	1582	CD2	TYR A			19.996	32.642	16.187		13.45
ATOM	1583	CE1	TYR A			20.224	32.320	18.933		13.15
ATOM	1584	CE2	TYR A			19.680	33.699	17.037		12.56
	1585	CZ	TYR A			19.801	33.530	18.404		13.22
MOTA						19.531	34.582	19.239		12.88
ATOM	1586	OH	TYR A				28.476	13.260		15.81
MOTA	1587	N	GLU A			18.664				17.54
ATOM	1588	CA	GLU A			18.741	27.586	12.081		
MOTA		C	GLU A			19.191	28.266			
MOTA	1590	0	GLU A			18.665	29.355	10.402		16.63
MOTA	1591	CB	GLU A	. 26	1	17.382	26.914	11.842		16.53
MOTA	1592	CG	GLU A	. 26	1	17.326	26.076	10.573	1.00	19.47
MOTA	1593	CD	GLU A	26	1	15.965	25.454	10.326		20.18
ATOM	1594		GLU A			14.956	26.037	10.766	1.00	21.27
MOTA	1595	OE2				15.902	24.390	9.673	1.00	20.94
ATOM	1596	N	VAL A			20.153	27.640	10.122	1.00	16.45
ATOM	1597	.CA	VAL A			20.679	28.147	8.842		16.13
	1598	C.	VAL A			20.620	27.006	7.831		17.33
	1599		VAL A			20.168	25.863	8.166		17.30
ATOM		O CD				22.131	28.624	8.982		14.58
ATOM	1600	CB	VAL A							14.84
ATOM	1601		VAL A			22.218	29.690	10.064		
ATOM	1602		VAL A			23.039	27.449	9.308		14.53
MOTA	1603	N	ILE P			21.064	27.271	6.608		17.34
MOTA	1604	CA	ILE A			21.044	26.245	5.554	1.00	
MOTA	1605	С	ILE A	26	3	22.419	26.042	4.931		16.64
MOTA	1606	0	ILE A	26	3	23.054	27.016	4.418	1.00	
MOTA	1607	CB	ILE A	26	3	20.031	26.619	4.445	1.00	
MOTA	1608	CG1	ILE A	. 26	3	18.608	26.522	4.996	1.00	18.90

MOTA	1609	CG2	ILE A	26	3 20.19	2 25.694	3.243	1.00 18.17
			ILE A					1.00 23.31
MOTA	1610	CD1						
MOTA	1611.	N	ILE A			7 24.802	4.988.	1.00 16.67
MOTA	1612	ĊA	ILE A	A 26	4 24.19	9 24.413	4.409	1.00 14.63
ATOM	1613	C	ILE 2				3.031	1.00 16.44
MOTA	1614	0	ILE A	A 26	23.01	9 22.915	2.908	1.00 13.53
ATOM.	1615	CB	ILE A	A 26	4 24.87	7 23.320	5.253	1.00 14.79
ATOM	1616	CG1					6.657	1.00 12.53
MOTA	1617		ILE A	1 26			4.563	1.00 12.07
ATOM	1618'	CD1	ILE A	1 26	4 25.68	5 22.799	7.615	1.00 12.69
ATOM	1619	N	VAL Z			6 24.334	1.992	1.00 17.37
ATOM	1620	CA	VAL A				0.627	1.00 18.64
MOTA	1621	С	VAL Z	1 26	5 25.36	8 23.004	0.006	1.00 19.95
ATOM	1622	0	VAL A	26	5 25.20	2 22.455	-1.127	1.00 19.29
		-					-0.322	1.00 18.56
MOTA	1623	CB	VAL A					
ATOM	1624	CG1	VAL A	26	5 22.87	4 25.901	0.287	1.00 16.70
ATOM	1625	CG2	VAL A	26	5 25.22	7 25.802	-0.590	1.00 17.47
	1626	N	ARG A				0.707	1.00 20.42
ATOM								
ATOM.	1627	CA	ARG A				0.165	1.00 20.48
ATOM	1628	С	ARG A	1 26	5 28,75	2 22.044	1.162	1.00 19.59
ATOM	1629	Ō	ARG A	26			1.885	1.00 19.51
MOTA	1630	CB	ARG A				-1.129	1.00 22.33
ATOM	1631	CG	ARG A	26	5 29.41	7 22.218	-1.713	1.00 22.40
ATOM	1632	CD	ARG A	26	29.93	9 23.170	-2.789	1.00 24.49
			ARG A				-3.322	1.00 24.49
MOTA	1633	NE						
MOTA	1634	cz	ARG A	26	31.44	4 22.266	-4.528	1.00 26.46
ATOM	1635	NH1	ARG A	26	30.42	6 22.061	-5.349	1.00 25.31
ATOM	1636	NH2	ARG A	26			-4.920	1.00 27.88
ATOM	1637	N	VAL A	26			1.246	1.00 18.31
ATOM	1638	CA	VAL A	26	7 30.56	1 20.766	2.136	1.00 18.32
MOTA	1639	С	VAL A	26			1.369	1.00 18.25
MOTA	1640	0	VAL A				0.489	1.00 19.14
ATOM	1641	CB	VAL A	26	7 30.248	3 19.974	3.456	1.00 18.72
ATOM	1642	CG1	VAL A	26	7 28.784	19.645	3.547	1.00 18.30
	1643	CG2					3.554	1.00 17.65
ATOM								
MOTA	1644	N	GLU A	. 26	32.90	3 20.471	1.647	1.00 16.18
MOTA	1645	CA	GLU F	26	34.046	5 19.848	0.990	1.00 17.71
ATOM	1646	C	GLU A	26	35.169	9 19.546	1.970	1.00 16.08
								1.00 13.62
ATOM	1647	0	GLU A				3.064	
MOTA	1648	CB	GLU A	26	34.550	20.717	-0.177	1.00 18.50
MOTA	1649	CG	GLU A	26	34.430	22.207	0.030	1.00 22.46
ATOM	1650	CD	GLU F				-1.181	1.00 22.13
MOTA	1651		GLU A					1.00 20.91
ATOM	1652	OE2	GLU A	. 26	35.927	7 23.703	-1.067	1.00 22.44
MOTA	1653	N	ILE A	. 26	35.948	3 18.531	1.623	1.00 13.57
ATOM	1654	CA	ILE A				2.418	1.00 13.89
MOTA	1655	C	ILE F				1.485	1.00 14.06
ATOM	1656	0	ILE A	. 26	38.396	17.832	0.386	1.00 14.03
MOTA	1657	CB	ILE A				2.703	1.00 14.48
							3.327	1.00 14.59
MOTA	1658		ILE F					
MOTA	1659	CG2	ILE F	. 26	38.180	16.193	3.645	1.00 12.12
MOTA	1660	CDİ	ILE F	26	35.358	3 17.022	4.592	1.00 13.16
	1661		ASN A				1.872	1.00 14.16
ATOM		И						
MOTA	1662	CA	ASN A	. 27			1.038	1.00 13.20
MOTA	1663	С	ASN A	. 27	39.774	20.177	-0.399	1.00 13.24
ATOM	1664	Ō	ASN A				-1.385	1.00 13.72
								1.00 11.19
ATOM	1665	CB	ASN A				1.047	
MOTA	1666	CG	ASN A	. 27	42.424	19.186	2.054	1.00 13.23
ATOM	1667	OD1	ASN A	. 27	42.339	20.224	2.790	1.00 13.62
ATOM	1668		ASN A				2.117	1.00 11.67
MOTA	1669	N	GLY A				-0.540	1.00 13.07
MOTA	1670	CA	GLY A	. 27	. 38.210	21.302	-1.858	1.00 13.58

MOTA	1671	С	GLY A	271	37.393	20.241	-2.564	1.00	14.87
MOTA	1672	0	GLY A	271	36.704	20.545	-3.581	1.00	13.70
MOTA	1673	N	GLN A		37.447	19.005	-2.076	1.00	14.64
MOTA	1674	CA	GLN A		36.674	17.914	-2.705	1.00	14.45
MOTA	1675	C	GLN A		35.261	17.870	-2.140	1.00	15.83
MOTA	1676	0	GLN A		35.050	17.717	-0.902	1.00	15.81
MOTA	1677	CB	GLN A		37.357	16.561	-2.486		14.85
MOTA	1678	CG	GLN A		36.692	15.421	-3.250		14.45
MOTA	1679	CD	GLN A		37.499	14.135	-3.211		16.34
MOTA	1680	OE:			37.097	13.134	-2.535		20.05
ATOM	1681	NE			38.633	14.121	-3.909		13.09
ATOM	1682	N	ASP A		34.291	17.995	-3.035		16.17
ATOM ATOM	1683 1684	CA C	ASP A 2		32.857 32.388	17.987 16.612	-2.686		17.89
ATOM	1685	0	ASP A 2		32.713	15.566	-2.201 -2.831		16.92
ATOM	1686	СВ	ASP A 2		32.060	18.395	-3.930		16.53 20.38
ATOM	1687	CG	ASP A 2		30.576	18.526	-3.665		20.89
ATOM	1688		ASP A 2		29.827	18.788	-4.630		21.98
ATOM	1689	OD2			30.155	18.378	-2.503		22.40
ATOM	1690	N	LEU A 2		31.639	16.576	-1.101		17.95
MOTA	1691	CA	LEU A 2	274	31.117	15.285	-0.587		19.37
ATOM	1692	C	LEU A 2	274	30.092	14.805	-1.598		21.18
MOTA	1693	0	LEU A 2	274	29.702	13.603	-1.623		20.08
ATOM	1694	CB	LEU A 2	274	30.451	15.455	0.783	1.00	18.46
MOTA	1695	CG	LEU A 2		31.356	15.595	2.011		19.89
MOTA	1696		LEU A 2		30.489	15.558	3.267	1.00	17.23
ATOM	1697	CD2			32.392	14.463	2.050		17.76
MOTA	1698	N	LYS A 2		29.646	15.736	-2.431		24.29
ATOM	1699	CA	LYS A 2		28.676	15.452	-3.501		29.08
ATOM	1700	C	LYS A 2		27.439	14.715	-3.000		28.92
ATOM ATOM	1701 1702	O CB	LYS A 2		27.119 29.360	13.586 14.642	-3.464		30.50
ATOM	1702	CG	LYS A 2		28.720	14.842	-4.608 -5.970		30.50 33.82
ATOM	1704	CD	LYS A 2		29.476	14.059	-7.042		36.63
ATOM	1705	CE.	LYS A 2		28.848	14.297	-8.408	1.00	
ATOM	1706	NZ	LYS A 2		28.742	15.759	-8.702	1.00	
ATOM	1707	N	MET A 2		26.734	15.329	-2.063		30.55
ATOM	1708	CA	MET A 2	•	25.519	14.722	-1.505	1.00	
ATOM	1709	С	MET A 2	76	24.319	15.592	-1.815	1.00	30.11
ATOM	1710	0	MET A 2	76	24.465	16.818	-2.117	1.00	28.94
MOTA	1711	CB	MET A 2		25.641	14.576	0.011	1.00	30.29
MOTA	1712	CG	MET A 2		26.706	13.605	0.469	1.00	
MOTA	1713	SD	MET A 2		26.687	13.418	2.261	1.00	
ATOM	1714	CE	MET A 2		25.174	12.457	2.477	1.00	
ATOM	1715	N	ASP A 2		23.136	14.994	-1.756	1.00	
ATOM ATOM	1716 1717	CA C	ASP A 2		21.906	15.750	-1.994	1.00	
ATOM	1717	0	ASP A 2		21.903 22.070	16.864	-0.955	1.00	
ATOM	1719	CB	ASP A 2		20.682	16.608 14.851	0.278 -1.818	1.00	
ATOM	1720	CG	ASP A 2		19.377	15.595	-2.029	1.00	
ATOM	1721		ASP A 2		18.332	14.925	-2.168	1.00	
ATOM	1722		ASP A 2		19.386	16.844	-2.049	1.00	
ATOM	1723	N	CYS A 2		21.732	18.089	-1.432	1.00	
ATOM	1724	CA	CYS A 2		21.725	19.294	-0.581	1.00	
ATOM	1725	C	CYS A 2		20.988	19.126	0.749	1.00	
MOTA	1726	ō	CYS A 2		21.503	19.540	1.834	1.00	
MOTA	1727	CB	CYS A 2		21.108	20.460	-1.362	1.00	
ATOM	1728	SG	CYS A 2		21.760	22.075	-0.852	1.00	
MOTA	1729	N	LYS A 2		19.802	18.529	0.705	1.00 3	
MOTA	1730	CA	LYS A 2		19.003	18.359	1.931	1.00	
MOTA	1731	С	LYS A 2		19.584	17.430	2.996	1.00 3	
MOTA	1732	0	LYS A 2	79	19.173	17.501	4.189	1.00 2	7.89

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MOTA	1733	CB	LYS	Α	279	17.574	17.939	1.567	1.00 34.74
MOTA	1734	CG	LYS			17.459	16.765	0.612	1.00 39.08
			LYS			17.576	15.429	1.326	1.00 41.32
MOTA	1735	CD							1.00 42.86
MOTA	1736	CE	LYS			17.185	14.289	0.393	
MOTA	1737	NZ	LYS	Α	279	17.118	12.978	1.099	1.00 45.07
MOTA	1738	N	GLU			20.525	16.570	2.621	1.00 27.06
						21.141	15.659	3.612	1.00 26.22
MOTA	1739	CA	GLU						-
MOTA	1740	C	GLΰ	Α	280	21.900	16.458	4.673	1.00 25.34
ATOM	1741	0	GLU	Α	280	21.920	16.074	5.886	1.00 23.01
ATOM	1742	CB	GLU			22.109	14.693	2.928	1.00 27.98
	_		GLU			21.459	13.725	1.946	1.00 31.24
MOTA	1743	CG						2.610	1.00 32.55
ATOM	1744	CD	GLU			20.486	12.765		
ATOM	1745	OE1	GLÜ	Α	280	20.447	12.704	3.857	1.00 33.21
ATOM	1746	OE2	GLU	Α	280	19.763	12.058	1.878	1.00 34.72
ATOM	1747	N	TYR			22.515	17.562	4.255	1.00 23.32
			TYR			23.295	18.420	5.176	1.00 22.69
MOTA	1748	CA						6.219	1.00 23.40
MOTA	1749	С	TYR			22.415	19.082		
MOTA	1750	0	TYR	Α	281	22.904		7.327	1.00 23.11
ATOM	1751	CB	TYR	A	281	24.035	19.515	4.400	1.00 20.26
ATOM	1752	CG	TYR	A	281	24.958	18.993	3.328	1.00 19.39
						25.858	17.961	3.601	1.00 17.78
ATOM	1753	CD1					19.534	2.042	1.00 18.55
MOTA	1754	CDS	TYR			24.943			
MOTA	17:55	CE1	TYR	А	281	26.719	17.478	2.623	1.00 17.05
ATOM	1756	CE2	TYR	A	281	25.808	19.058	1.051	1.00 18.53
ATOM	1757	CZ	TYR			26.692	18.028	1.355	1.00 17.87
		OH	TYR			27.558	17.533	0.407	1.00 18.13
ATOM	1758						19.232	5.899	1.00 22.82
MOTA		N	ASN			21.136			
MOTA	1760	CA	ASN	Α	282	20.194	19.881	6.820	1.00 23.17
MOTA	1761	С	ASN	Α	282	19.089	18.922	7.238	1.00 23.84
ATOM	1762	Ō	ASN			17.987	19.366	7.685	1.00 21.83
	•		ASN			19.598	21.111	6.137	1.00 22.42
MOTA	1763	CB						5.549	1.00 23.90
MOTA	1764	CG	ASN			20.665	22.018		
ATOM	1765	OD1	ASN	Α	282	21.426	22.693	6.298	1.00 23.87
MOTA	1766	ND2	ASN	A	282	20.760	22.044	4.224	1.00 23.36
ATOM	1767	N	TYR			19.343	17.623	7.102	1.00 25.74
						18.322	16.633	7.472	1.00 28.01
MOTA	1768	CA			283			8.912	1.00 29.29
MOTA	1769	C			283	17.905	16.843		
ATOM	1770	0			283	18.686	16.572	9.881	1.00 27.50
MOTA	1771	CB	TYR	A	283	18.810	15.200	7.280	1.00 29.52
ATOM	1772	CG			283	17.783	14.200	7.756	1.00 31.64
	1773	CD1			283	16.428	14.374	7.460	1.00 32.38
ATOM						18.153	13.098	8.523	1.00 33.44
ATOM	1774	CD2			283				1.00 33.96
ATOM	1775	CE1				15.468	13.479	7.919	
MOTA	1776	CE2	TYR	Α	283	17.201	12.194	8.987	1.00 35.48
ATOM	1777	CZ			283	15.860	12.392	8.683	1.00 35.35
ATOM	1778	OH			283	14.918	11.504	9.149	1.00 36.54
					284	16.665	17.299	9.043	1.00 30.23
MOTA	1779	N						10.312	1.00 28.41
MOTA	1780	CA			284	16.026	17.638		
MOTA	1781	С	ASP	Α	284	16.273	19.129	10.409	1.00 27.12
ATOM	1782	0	ASP	A	284	15.309	19.953	10.305	1.00 25.19
ATOM	1783	CB			284	16.684	16.928	11.494	1.00 33.07
						16.035	17.283	12.813	1.00 33.49
MOTA	1784	CG			284				1.00 37.38
MOTA	1785		ASP			16.520	16.815	13.860	
MOTA	1786	OD2	ASP	Α	284	15,035	18.031	12.802	1.00 35.95
ATOM	1787	N			285	17.542	19.499	10.563	1.00 22.62
		CA			285	17.914	20.927	10.678	1.00 20.42
MOTA	1788						21.145	10.812	1.00 19.89
MOTA	1789	С			285	19.420			1.00 19.63
MOTA	1790	0			285	20.209		11.037	
ATOM	1791	CB	LYS	A	285	17.230	21.540	11.903	1.00 18.63
ATOM	1792	CG			285	17.753	20.987	13.232	1.00 16.63
	1793	CD			285	16.966		14.421	1.00 14.93
ATOM					285	17.551	21.088	15.754	1.00 15.57
MOTA	1794	CE	ГXS	A	200	11.771	22.000		

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MOTA	1795	NZ	LYS	Α	285	17.482	19.606	15.974	1.00 13.50
	1796				286	19.827	22.402		
ATOM		N						10.678	1.00 17.19
ATOM	1797.	CA	SER	Α	286	21.241	22.808	10.827	1.00 16.52
ATOM	1798	C	SER	Α	286	21.228	24.034	11.727	1.00 15.74
MOTA	1799	0	SER	A	286	20.592	25.080	11.377	1.00 14.46
ATOM	1800	CB	SER	Α	286	21.862	23.179	9.475	1.00 16.90
ATOM	1801	OG	SER			22.064	22.036	8,671	1.00 16.60
MOTA	1802	N	ILE	Α	287	21.900	23.946	12.870	1.00 13.25
ATOM	1803	CA	ILE	Α	287	21.933	25.079	13.805	1.00 13.97
ATOM	1804	С	ILE			23.342	25.511	14.206	1.00 15.14
MOTA	1805	0	ILE	Α	287	24.346	24.750	14.024	1.00 14.63
ATOM	1806	CB	ILE	Δ	287	21.145	24.757	15.102	1.00 13.55
ATOM	1807	CG1				21.898	23.717	15.929	1.00 12.52
MOTA	1808	CG2	ILE	Α	287	19.758	24.214	14.754	1.00 12.10
ATOM	1809	CD1	ILE	Α	287	21.274	23.455	17.283	1.00 14.43
ATOM	1810	N	VAL			23.431	26.728	14.732	1.00 14.78
ATOM	1811	CA	VAL	Α	288	24.701	27.292	15.223	1.00 15.54
ATOM	1812	С	VAL	Α	288	24.510	27.262	16.733	1.00 16.05
			VAL				27.930		
ATOM	1813	0.				23.571			1.00 15.61
ATOM	1814	CB	VAL	A	288	24.896	28.751	14.767	1.00 15.19
ATOM	1815	CG1	VAL	Α	288	26.248	29.259	15.239	1.00 14.78
	1816							13.246	1.00 15.19
MOTA			VAL			24.791	28.842		
ATOM	1817	N	ASP	Α	289	25.355	26.512	17.430	1.00 15.91
MOTA	1818	CA	ASP	Α	289	25.194	26.373	18.891	1.00 14.81
			ASP			26.467	26.444	19.724	
MOTA	1819	С							1.00 15.27
MOTA	1820	0	ASP	Α	289	27.322	25.504	19.700	1.00 15.75
ATOM	1821	CB	ASP	Α	289	24.467	25.060	19.168	1.00 12.65
		CG					24.806		1.00 13.29
MOTA	1822		ASP			24.264		20.634	
ATOM	1823	ODl	ASP	Α	289	24.372	25.768	21.426	1.00 11.88
MOTA	1824	OD2	ASP	Α	289	23.981	23.639	20.988	1.00 10.63
	1825	N	SER			26.604	27.529	20.479	1.00 15.19
MOTA									
ATOM	1826	CA	SER	Α	290	27.782	27.730	21.346	1.00 14.55
ATOM	1827	С	SER	Α	290	27.770	26.748	22.510	1.00 15.43
	1828		SER			28.823	26.539	23.186	1.00 13.77
MOTA		0							
ATOM	1829	CB	SER	Α	290	27.795	29.165	21.888	1.00 15.33
ATOM	1830	OG	SER	Α	290	26.614	29.442	22.620	1.00 12.79
	1831		GLY			26.612	26.137	22.759	1.00 14.34
ATOM		N							
ATOM	1832	CA	GLY			26.486	25.192	23.856	1.00 14.93
ATOM	1833	С	GLY	Α	291	26.779	23.751	23.479	1.00 16.64
ATOM	1834	ō	GLY			26.502	22.792	24.277	1.00 14.49
MOTA	1835	N	THR			27.305	23.556	22.277	1.00 16.47
ATOM	1836	CA	THR	Α	292	27.674	22.202	21.812	1.00 15.30
MOTA	1837	С	THR			29.159			1.00 14.67
ATOM	1838	0	THR			29.653	23.102	20.725	1.00 13.26
ATOM	1839	CB	THR	Α	292	26.889	21.784	20.550	1.00 15.29
MOTA	1840	OG1	THR	Α	292	25.522	21.521	20.895	1.00 13.88
MOTA	1841		THR			27.514	20.527	19.932	1.00 13.59
MOTA	1842	N	THR	Α	293	29.887	21.253	22.027	1.00 14.43
MOTA	1843	CA	THR	A	293	31.343	21.162	21.801	1.00 12.76
			THR				20.906	20.348	1.00 14.47
MOTA	1844	С							
ATOM	1845	0	THR	A	293	32.478	21.735	19.712	1.00 14.61
MOTA	1846	CB	THR	A	293	31.949	20.035	22.650	1.00 12.36
MOTA	1847		THR			31.726	20.304	24.041	1.00 10.79
MOTA	1848	CG2	THR	Α	293	33.437	19.916	22.382	1.00 9.56
ATOM	1849	N	ASN	Α	294	31.286	19.783	19.810	1.00 13.53
									1.00 15.26
ATOM	1850	CA	ASN			31.648	19.349	18.440	
MOTA	1851	С	ASN			30.871	19.917	17.276	1.00 15.45
ATOM	1852	0	ASN	A	294	29.851	20.662	17.431	1.00 13.68
			ASN				17.832	18.307	1.00 14.81
ATOM	1853	CB				31.494			
MOTA	1854	CG	ASN			32.351	17.051	19.270	1.00 14.13
MOTA	1855	OD1	ASN	A	294	32.264	15.791	19.304	1.00 19.85
MOTA	1856		ASN			33.174	17.734	20.051	1.00 13.25
AIOM	1000	14174	WOTA .		~~3	JJ.114	21.133	20.022	20.00

MOTA	1857	N	LEU A	295	31.365	19.556	16.096	1.00 15.21
ATOM	1858	CA	LEU A		30,689	19.866	14.835	1.00 15.29
MOTA	1859.	С	LEU A		29.924	18.548	14.719	1.00 16.43
ATOM	1860	0	LEU A	295	30.556	17.452	14.575	1.00 16.34
MOTA	1861	CB	LEU A	295	31.674	19.963	13.671	1.00 13.54
MOTA	1862	CG	LEU A	295	31.017	19.837	12.287	1.00 14.74
ATOM	1863		LEU A		29.991	20.947	12.109	1.00 14.37
MOTA	1864	CD2	LEU A		32.073	19.903	11.179	1.00 13.91
ATOM	1865	N	ARG A	296	28.606	18.591	14.831	1.00 16.08
MOTA	1866	CA	ARG A	296	27.827	17.349	14.719	1.00 17.47
MOTA	1867	С	ARG A	296	27.180	17.300	13.343	1.00 17.04
ATOM	1868	Ō	ARG A		26.655	18.339	12.840	
							15.834	1.00 18.37
ATOM'	1869'	CB	ARG A		26.785	17.290		
MOTA	1870	CG	ARG A		27.421	17.444	17.208	1.00 19.73
MOTA	1871	CD	ARG A	296	26.425	17.262	18.324	1.00 22.63
ATOM	1872	NE	ARG A	296	26.292	15.867	18.722	1.00 25.23
MOTA	1873	CZ	ARG A	296	25.135	15.223	18.776	1.00 26.52
ATOM	1874	NH1			24.011	15.851	18.446	1.00 27.11
ATOM	1875	NH2			25.100	13.961	19.179	1.00 27.00
MOTA	1876	N	LEU A		27.211	16.123	12.722	1.00 15.65
ATOM	1877	CA	LEU A		26.660	15.945	11.356	1.00 15.33
MOTA	1878	C	LEU A	297	25.657	14.800	11.246	1.00 17.46
ATOM	1879	0	LEU A	297	25.795	13.743	11.938	1.00 16.37
MOTA	1880	СВ	LEU A	297	27.806	15.681	10.371	1.00 12.00
ATOM	1881	CG	LEU A		28.925	16.729	10.277	1.00 11.84
	1882		LEU A		30.136	16.148	9.561	1.00 8.16
ATOM								
ATOM	1883	CD2			28.410	17.962	9.559	
MOTA	1884	N	PRO A		24.636	14.960	10.386	1.00 19.11
MOTA	1885	CA	PRO A	298	23.636	13.901	10.217	1.00 20.53
MOTA	1886	С	PRO A	298	24.387	12.619	9.868	1.00 21.03
MOTA	1887	0	PRO A	298	25.419	12.668	9.131	1.00 21.77
ATOM	1888	СВ	PRO A		22.788	14.411	9.054	1.00 19.18
ATOM	1889	CG	PRO A		22.861	15.897	9.209	1.00 20.46
					24.335	16.111	9.517	1.00 20.40
MOTA	1890	CD	PRO A					
MOTA	1891	N	LYS A		23.911	11.487	10.376	1.00 22.77
ATOM	1892	CA	LYS A		24.562	10.169	10.137	1.00 25.34
MOTA	1893	С	LYS A	299	25.169	9.979	8.753	1.00 24.56
ATOM	1894	0	LYS A	299	26.393·	9.681	8.617	1.00 22.24
ATOM	1895	CB	LYS A	299	23.566	9.034	10.387	1.00 29.05
ATOM	1896	CG	LYS A		24.156	7.650	10.146	1.00 33.27
ATOM	1897	CD	LYS A		23.144	6.547	10.408	1.00 37.10
			LYS A			5.178	10.151	1.00 38.78
MOTA	1898	CE		-	23.758			
MOTA	1899	NZ	LYS A		22.775	4.077	10.380	1.00 42.51
ATOM	1900	N	LYS A		24.340	10.127	7.729	1.00 24.24
MOTA	1901	CA	LYS A	300	24.774	9.955	6.333	1.00 25.41
MOTA	1902	С	LYS A	300	25.901	10.916	5.952	1.00 24.12
MOTA	1903	0	LYS A	300	26.889	10.515	5.262	1.00 23.67
ATOM	1904	CB	LYS A		23.576	10.154	5.403	1.00 28.77
ATOM	1905	CG	LYS A		23.788	9.660	3.990	1.00 33.37
							3.569	1.00 38.01
MOTA	1906	CD	LYS A		22.661	8.718		
MOTA	1907	CE	LYS A		21.298	9.393	3.652	1.00 40.18
MOTA	1908	NZ	LYS A	300	20.191	8.455	3.291	1.00 42.69
ATOM	1909	N	VAL A	301	25.784	12.172	6.368	1.00 20.46
MOTA	1910	CA	VAL A	301	26.832	13.169	6.058	1.00 18.21
ATOM	1911	C	VAL A		28.083	12.842	6.867	1.00 17.93
ATOM	1912	ō	VAL A		29.241	12.929	6.343	1.00 16.84
			VAL A		26.358	14.601	6.391	1.00 17.29
ATOM	1913	CB					6.105	1.00 17.23
ATOM	1914		VAL A		27.468	15.605		
MOTA	1915		VAL A		25.118	14.935	5.565	1.00 16.34
MOTA	1916	N	PHE A		27.887	12.448	8.122	1.00 17.43
MOTA	1917	CA	PHE A		29.032	12.099	8.990	1.00 18.16
MOTA	1918	С	PHE A	302	29.854	10.957	8.399	1.00 18.95

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ATOM	1919	0	PHE A	302	31.121	11.004	8.399	1.00 18.60
ATOM	1920	CB	PHE A		28.550	11.713	10.391	1.00 17.38
MOTA	1921 -	CG	PHE A		29.639	11.180	11.265	1.00 19.16
MOTA	1922	CD1			29.866	9.810	11.362	1.00 17.81
MOTA	1923	CD2	PHE A		30.498	12.051	11.923	1.00 18.89
ATOM	1924	CE1	PHE A		30.934	9.320	12.096	1.00 19.63
	1925	CE2	PHE A		31.573	11.569	12.660	1.00 19.90
MOTA					31.793	10.201	12.747	1.00 19.13
ATOM	1926	CZ	PHE A					1.00 19.10
MOTA	1927	Ŋ	GLU A		29.172	9.931	7.901	
MOTA	1928	CA	GLU A		29.859	8.769	7.295	
MOTA	1929	С	GLU A		30.679	9.189	6.083	1.00 19.19
MOTA	1930	0	GLU A		31.865	8.777	5.929	1.00 18.04
ATOM	1931	CB	GLU A		28.836	7.704	6.888	1.00 24.72
MOTA	1932	CG	GLU A		28.246	6.939	8.069	1.00 29.90
ATOM	1933	CD	GLU A	303	27.051	6.076	7.683	1.00 33.77
ATOM	1934	OE1	GLU A		26.585	5.294	8.541	1.00 36.31
ATOM	1935	OE2	GLU A	303	26.572	6.183	6.528	1.00 36.51
ATOM	1936	N	ALA A	304	30.088	9.998	5.216	1.00 17.86
ATOM	1937	CA	ALA A	304	30.805	10.472	4.007	1.00 18.11
MOTA	1938	С	ALA A	304	31.999	11.354	4.386	1.00 17.49
ATOM	1939	0	ALA A	304	33.102	11.242	3.777	1.00 17.76
MOTA	1940	CB	ALA A	304	29.849	11.244	3.102	1.00 17.14
ATOM	1941	N	ALA A	305	31.812	12.221	5.377	1.00 17.06
ATOM	1942	CA	ALA A		32.900	13.128	5.829	1.00 16.43
ATOM	1943	C	ALA A		34.092	12.387	6.440	1.00 16.39
ATOM	1944	ō	ALA A		35.272	12.644	6.054	1.00 17.78
ATOM	1945	-	ALA A		32.351	14.140	6.833	1.00 15.92
ATOM	1946	N	VAL A		33.842	11.476	7.375	1.00 15.50
ATOM	1947	CA	VAL A		34.971	10.756	8.004	1.00 17.31
ATOM	1948	C	VAL A		35.719	9.920	6.987	1.00 16.95
ATOM	1949	Ö	VAL A		36.983	9.829	7.029	1.00 16.21
	1950	CB	VAL A		34.514	9.845	9.162	1.00 17.93
ATOM	1951	CG1			33.954	10.693	10.280	1.00 19.37
MOTA			VAL A		33.477	8.851	8.669	1.00 19.63
ATOM	1952		LYS A		34.987	9.307	6.065	1.00 17.11
MOTA	1953	N	LYS A		35.641	8.488	5.032	1.00 18.39
ATOM	1954	CA			36.654	9.350	4.279	1.00 17.59
ATOM	1955	C	LYS A		37.848	8.959	4.107	1.00 18.09
MOTA	1956	0	LYS A		34.602	7.940	4.052	1.00 19.72
ATOM	1957	CB	LYS A		35.212	7.112	2.930	1.00 24.02
MOTA	1958	CG	LYS A		34.147	6.415	2.102	1.00 26.72
MOTA	1959	CD	LYS A			5.505	1.058	1.00 29.36
ATOM	1960	CE	LYS A		34.779			
MOTA	1961	NZ	LYS A		33.745	4.869	0.193 3.842	1.00 31.68
ATOM	1962	N	SER A		36.205	10.520	3.042	1.00 17.46
MOTA	1963	CA	SER A		37.059	11.460		1.00 17.40
MOTA	1964	C	SER A		38.198	12.000	3.953	1.00 10.11
MOTA	1965	0	SER A		39.378	12.056	3.501	
MOTA	1966	CB	SER A		36.208	12.620	2.560	
MOTA	1967	OG	SER A		36.982	13.505	1.774	1.00 19.76
MOTA	1968	N	ILE A		37.886	12.400	5.180	1.00 16.07
MOTA	1969	CA	ILE A		38.926	12.927	6.083	1.00 14.41
MOTA	1970	Ċ	ILE A		39.945	11.831	6.378	1.00 14.93
MOTA	1971	0	ILE A		41.171	12.112	6.505	1.00 14.90
MOTA	1972	CB	ILE A	. 309	38.310	13.439	7.401	1.00 13.88
ATOM	1973	CG1	ILE A	. 309	37.346	14.595	7.099	1.00 13.08
ATOM	1974	CG2	ILE A	309	39.404	13.887	8.350	1.00 11.40
MOTA	1975	CD1	ILE A	309	36.575	15.084	8.315	1.00 12.70
MOTA	1976	N	LYS A		39.475	10.592	6.485	1.00 15.62
MOTA	1977	CA	LYS A		40.375	9.437	6.752	1.00 17.74
MOTA	1978	С	LYS A		41.289	9.223	5.559	1.00 17.22
ATOM	1979	0	LYS A		42.532	9.061	5.715	1.00 16.87
ATOM	1980	CB	LYS A		39.577	8.149	6.976	1.00 18.35
						_		

ATOM	1981	CG	LYS A	310	39.003	7.953	8.373	1.00 20.85
								_
ATOM	1982	CD	LYS A		38.269	6.617	8.432	1.00 22.02
MOTA	1983	CE	LYS A	310	37.584	6.404	9.75 <b>7</b>	1.00 25.26
MOTA	1984	NZ	LYS 2	310	36.808	5.129	9.752	1.00 26.15
MOTA	1985	N	ALA A		40.698	9.211	4.370	1.00 15.56
ATOM	1986	CA	ALA A	311	41.466	9.007	3.124	1.00 17.77
MOTA	1987	С	ALA A		42.549	10.071	2.990	1.00 17.36
MOTA	1988	0	ALA A	311	43.708	9.768	2.578	1.00 20.71
ATOM	1989	СВ	ALA A	311	40.524	9.047	1.908	1.00 14.11
					42.210	11.309	3.330	1.00 16.63
MOTA	1990	N	ALA A					
MOTA	1991	CA	ALA A	312	43.184	12.418	3.235	1.00 15.73
MOTA	1992 -	С	ALA A	312	44.247	12.342	4.333	1.00 15.59
						12.958	4.207	1.00 13.09
MOTA	1993	0	ALA A		45.348			
ATOM	1994	CB	ALA A	312	42.449	13.758	3.301	1.00 13.50
ATOM	1995	N	SER A	313	43.950	11.593	5.393	1.00 17.05
					44.867	11.432	6.560	1.00 19.05
MOTA	1996	CA	SER A					
ATOM	1997	С	SER A	313	45.579	10.085	6.593	1.00 19.49
ATOM	1998	0	SER A	313	46.332	9.787	7.568	1.00 21.95
					44.075	11.555	7.865	1.00 17.23
MOTA	1999	CB	SER A					
MOTA	2000	OG	SER A	313	43.501	12.834	8.003	1.00 23.58
ATOM	2001	N	SER A	314	45.368	9.270	5.570	1.00 20.76
			SER A		45.952	7.909	5.513	1.00 22.73
MOTA	2002	CA						
ATOM	2003	C	SER A	314	47.436	7.725	5.838	1.00 21.90
ATOM	2004	0	SER A	314	47.825	6.639	6.359	1.00 20.76
					45.650	7.271	4.150	1.00 22.50
MOTA	2005	CB	SER A					
ATOM	2006	OG	SER A	314	46.207	8.032	3.093	1.00 27.94
ATOM	2007	N	THR A	315	48.285	8.714	5.570	1.00 20.90
					49.732	8.523	5.868	1.00 23.78
MOTA	2008	CA	THR A					
ATOM	2009	С	THR A	315	50.020	8.454	7.361	1.00 25.42
ATOM	2010	0	THR A	315	51.191	8.219	7.784	1.00 26.24
	2011		THR A		50.616	9.634	5.257	1.00 23.59
MOTA		CB						•
ATOM	2012	OG1	THR A	315	50.256	10.901	5.818	1.00 22.73
ATOM	2013	CG2	THR A	315	50.456	9.668	3.745	1.00 22.59
	2014	N	GLU A		48.994	8.655	8.176	1.00 27.46
MOTA								
MOTA	2015	$^{ca}$	GLU A	316	49.170	8.589	9.638	1.00 29.81
ATOM	2016	С	GLU A	316	48.258	7.503	10.201	1.00 30.55
ATOM	2017	Ō	GLU A		47.110	7.314	9.710	1.00 29.51
MOTA	2018	CB	GLU A		48.819	9.931	10.279	1.00 32.51
ATOM	2019	CG	GLU A	316	49.277	10.039	11.725	1.00 36.72
ATOM	2020	CD	GLU A		50.571	10.818	11.879	1.00 36.99
								1.00 37.39
MOTA	2021	OE1			51.456	10.728	11.003	
MOTA	2022	OE2	GLU A	316	50.704	11.522	12.893	1.00 41.14
MOTA	2023	N	LYS A	317	48.736	6.775	11.205	1.00 32.69
			LYS A		47.928	5.702	11.828	1.00 35.09
MOTA	2024	CA						
MOTA	2025	С	LYS A	317	47.216	6.223	13.071	1.00 33.44
ATOM	2026	0	LYS A	317	47.804	7.005	13.883	1.00 34.13
	2027	CB	LYS A		48.809	4.505	12.202	1.00 38.52
MOTA								
MOTA	2028	CG	LYS A	317	49.980	4.844	13.106	1.00 43.41
MOTA	2029	CD	LYS A	317	50.665	3.588	13.638	1.00 46.99
MOTA	2030	CE	LYS A		51.165	2.686	12.514	1.00 48.65
MOTA	2031	NZ	LYS A	317	51.731	1.410	13.043	1.00 49.49
ATOM	2032	N	PHE A	318	45.965	5.818	13.245	1.00 31.00
	2033	CA	PHE A		45.188	6.272	14.408	1.00 30.33
ATOM								
MOTA	2034	С	PHE A	318	44.683	5.120	15.263	1.00 30.57
MOTA	2035	0	PHE A	318	44.171	4.088	14.732	1.00 29.80
ATOM	2036	CB	PHE A		44.014	7.135	13.944	1.00 28.83
MOTA	2037	CG	PHE A		44.436	8.367		1.00 28.31
ATOM	2038	CD1	PHE A	318	44.625	8.333	11.817	1.00 27.09
ATOM	2039		PHE A		44.686	9.554	13.879	1.00 27.59
MOTA	2040		PHE A		45.060	9.466	11.130	1.00 27.37
MOTA	2041	CE2	PHE A	318	45.122	10.691	13.200	1.00 26.98
ATOM	2042	CZ	PHE A		45.309	10.648	11.826	1.00 27.12
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ATOM	2043	N	PRO	Α	319		44.805	5.252	16.591	1.00	30.02
MOTA	2044	CA	PRO	Α	319		44.361	4.222	17.535	1.00	30.20
MOTA	2045.	С	PRO	Α	319		42.864	3.977	17.460	1.00	29.88
ATOM	2046	0	PRO	Α	319		42.087	4.882	17.040	1.00	29.27
ATOM	2047	CB	PRO				44.777	4.793	18.890	1.00	30.49
ATOM	2048	CG	PRO				44.667	6.276	18.674		31.99
ATOM	2049	CD	PRO				45.308	6.437	17.309		30.77
ATOM	2050	N	ASP				42.449	2.779	17.860		30.77
ATOM	2051	CA	ASP				41.018	2.389	17.867		29.79
ATOM	2052	C	ASP				40.183	3.406	18.652		28.71
ATOM	2053	0	ASP				40.560	3.804	19.804		27.90
MOTA	2054	CB	ASP				40.855	1.009	18.520		31.81
MOTA	2055	CG	ASP				41.545	-0.104	17.740		34.27
ATOM	2056		ASP				41.787	-1.182	18.331		34.13
MOTA	2057	OD2	ASP	Α	320		41.833	0.092	16.538	1.00	35.41
ATOM	2058	N	GLY	Α	321		39.067	3.837	18.068	1.00	26.34
MOTA	2059	CA	GLY	Α	321		38.193	4.781	18.745	1.00	24.91
ATOM	2060	С	GLY	Α	321		38.439	6.259	18.490	1.00	23.96
MOTA	2061	0	GLY	Α	321	•	37.632	7.129	18.941	1.00	23.66
MOTA	2062	N	PHE	Α	322		39.519	6.591	17.793	1.00	22.07
ATOM	2063	CA	PHE	Α	322		39.810	8.011	17.507	1.00	20.41
ATOM	2064	C	PHE				38.705	8.670	16.684		20.53
ATOM	2065	ō	PHE				38.157	9.743	17.078		20.75
ATOM	2066	CB	PHE				41.126	8.157	16.747		19.07
ATOM	2067	CG	PHE				41.405	9.567	16.306		19.05
ATOM	2068	CD1	PHE				41.701	10.555	17.240		17.04
MOTA	2069	CD2	PHE				41.326	9.918	14.960		17.20
											18.99
ATOM	2070	CE1	PHE				41.912	11.872	16.840		
ATOM	2071	CE2	PHE				41.535	11.229	14.552		17.99
MOTA	2072	CZ	PHE				41.829	12.210	15.494		16.28
MOTA	2073	N	TRP				.38.367	8.063	15.552		20.75
MOTA	2074	CA	TRP				37.330	8.622	14.664		22.37
ATOM	2075	С	TRP				35.940	8.626	15.273		23.50
MOTA	2076	Ο,	TRP				35.036	9.379	14.804		22.84
MOTA	2077	CB	TRP				37.322	7.872	13.335		21.45
MOTA	2078	CG	TRP				38.643	7.924	12.664		20.71
MOTA	2079	CD1	TRP	A	323		39.566	6.921	12.594	1.00	20.50
ATOM	2080	CD2	TRP	A	323		39.217	9.049	11.986	1.00	20.31
MOTA	2081	NE1	TRP	Α	323		40.679	7.349	11.913	1.00	20.18
MOTA	2082	CE2	TRP	A	323		40.492	8.651	11.527	1.00	20.95
ATOM	2083	CE3	TRP	Α	323		38.778	10.354	11.722	1.00	20.80
MOTA	2084	CZ2	TRP	A	323		41.337 -	9.511	10.816	1.00	20.49
MOTA	2085	CZ3	TRP	Α	323		39.618	11.212	11.013	1.00	21.58
ATOM	2086	CH2	TRP .				40.885	10.784	10.569	1.00	21.15
MOTA	2087	N.	LEU .	Α	324		35.734	7.810	16.300	1.00	26.13
ATOM	2088	CA	LEU				34.428	7.772	16.983		27.96
ATOM	2089	С	LEU				34.417	8.877	18.040	1.00	
MOTA	2090	ō	LEU				33.413	9.044	18.799	1.00	
ATOM	2091	СB	LEU				34.202	6.408	17.642	1.00	
MOTA	2092	CG	LEU				33.910	5.236	16.697	1.00	
ATOM	2093		LEU .				33.791	3.948	17.501	1.00	
ATOM	2094		LEU .				32.625	5.499	15.924	1.00	
ATOM	2095	in	GLY .				35.513	9.634	18.098	1.00	
MOTA	2096	CA	GLY .				35.632	10.728	19.048	1.00	
MOTA	2097	C	GLY .				35.794	10.280	20.489	1.00	
ATOM	2098	0	GLY .				35.687	11.109	21.442	1.00	
ATOM	2099	N	GLU .				36.067	8.995	20.683	1.00	
	2100	CA	GLU .				36.225	8.436	22.042	1.00	
ATOM	2101	С	GLU .				37.655	8.482	22.563		33.56.
	2102	0	GLU .				37.907	8.933	23.720	1.00	
MOTA	2103	CB	GLU .				35.728	6.992	22.062	1.00	
ATOM	2104	CG	GLU .	A	326		34.267	6.847	21.683	1.00	38.03

ATOM	2105	CD	GLU	Α	326	33.855	5.401	21.494	1.00	40.36
ATOM	2106	OE1	GLU	Δ	326	32.662	5.162	21.207	1 00	41.84
								21.626		42.10
MOTA	2107.	OE2				34.720	4.506			
MOTA	2108	N	${\tt GLN}$	Α	327	38.602	8.031	21.750	1.00	32.81
ATOM	2109	CA	GLN	Α	327	40.009	8.017	22.178	1.00	31.36
						40.844	9.142	21.608		30.14
MOTA	2110	C			327					
ATOM	2111	0	$\operatorname{GLN}$	Α	327	40.612	9.626	20.458	1.00	28.97
MOTA	2112	CB	GLN	Α	327	40.650	6.667	21.842	1.00	34.41
ATOM	2113	CG			327	40.770	5.749	23.060		38.96
MOTA	2114	CD	GLN	Α	327	39.443	5.546	23.778		40.61
ATOM	2115	OE1	GLN	A	327	39.410	5.223	25.002	1.00	42.73
MOTA	2116	NE2		Δ	327	38.344	5.714	23.053	1.00	42.75
MOTA	2117	Ŋ	LEU			41.814	9.581	22.394		28.01
ATOM	2118	CA	LEU	Α	.328	42.695	10.663	21.964	1.00	28.64
MOTA	2119	С	LEU	Α	328	43.889	10.100	21.219	1.00	27.50
ATOM	2120	Õ	LEU			44.207	8.873	21.317		27.23
MOTA	2121	CB	LEU			43.177	11.467	23.180		29.39
MOTA	2122	CG	LEU	Α	328	43.924	10.735	24.304	1.00	31.09
MOTA	2123	CD1	LEU	Α	328	45.298	10.283	23.831	1.00	31.75
ATOM	2124	CDS	LEU	Δ	328	44.074	11.669	25.498	1 00	31.12
ATOM	2125	N	VAL			44.539	10.961	20.449		25.26
MOTA	2126	CA	VAL	Α	329	45.748	10.583	19.722	1.00	23.64
MOTA	2127	С	VAL	Α	329	46.779	11.593	20.203	1.00	23.76
ATOM	2128	ō	VAL			46.431	12.786	20.476		21.96
MOTA	2129	CB	VAL			45.560	10.675	18.194		23.82
MOTA	2130	CG1	VAL	Α	329	45.100	12.070	17.794	1.00	23.64
ATOM	2131	CG2	VAL	Α	329	46.866	10.317	17.501	1.00	23.70
	2132	N	CYS			48.025	11.157	20.344		23.69
ATOM										
MOTA	2133	CA	CYS			49.088	12.046	20.830	T-00	24.17
ATOM	2134	С	CYS	Α	330	50.315	12.060	19.937	1.00	23.87
ATOM	2135	0	CYS	Δ	330	50.592	11.089	19.165	1.00	24.32
						49.548	11.633	22.228		24.93
MOTA	2136	CB	CYS							
MOTA	2137	SG	CYS	Α	330	48.353	11.638	23.608	1.00	29.07
ATOM	2138	N	TRP	Α	331	51.069	13.144	20.047	1.00	22.66
ATOM	2139	CA	TRP	Δ	331	52.306	13.318	19.281	1.00	22.40
						53.333	13.972	20.177		22.22
ATOM	2140	C	TRP							
MOTA	2141	0	TRP			52.979	14.698	21.154		21.57
MOTA	2142	CB	TRP	Α	331	52.069	14.207	18.064	1.00	21.16
MOTA	2143	CG	TRP	Α	331	51.345	13.524	16.959	1.00	19.61
			TRP			51.868	12.634	16.067	1.00	18.33
ATOM	2144									
MOTA	2145	CD2	TRP			49.966	13.684	16.606	1.00	18.42
ATOM	2146	NE1	TRP	Α	331	50.902	12.233	15.177	1.00	17.37
MOTA	2147	CE2	TRP	A	331	49.721	12.862	15.488	1.00	18.60
	2148		TRP			48.911	14.446	17.130	1 00	19.20
ATOM										
ATOM	2149		TRP			48.467	12.778	14.874		17.86
MOTA	2150	CZ3	TRP	Α	331	47.659	14.364	16.521	1.00	19.94
MOTA	2151	CH2	TRP	Α	331	47.450	13.535	15.406	1.00	19.08
			GLN		333	54.598	13.730	19.873		23.04
MOTA	2152	N								
MOTA	2153	CA	GLN			55.689	14.321	20.648		25.14
MOTA	2154	Ç	GLN	Α	332	55.490	15.836	20.594	1.00	23.64
MOTA	2155	0	GLN	Α	332	55.066	16.397	19.533	1.00	23.11
			GLN			57.020	13.937	20.015		27.80
MOTA	2156	CB								
MOTA	2157	ĊG	GLN			58.171	13.877	20.982		33.30
MOTA	2158	CD	GLN	Α	332	59.450	13.445	20.305	1.00	35.55
ATOM	2159		GLN			60.060	14.224	19.507	1.00	36.94
										36.57
MOTA	2160		GLN			59.879	12.217	20.579		
ATOM	2161	N	ALA			55.778	16.506	21.704		22.79
MOTA	2162	CA	ALA	A	333	55.618	17.977	21.820	1.00	21.04
ATOM	2163	C	ALA			55.936	18.759	20.552		19.77
										19.85
MOTA	2164	0	ALA			57.076	18.671	19.997		
MOTA	2165	CB	ALA				18.499	22.971		21.00
MOTA	2166	N	GLY	Α	334	54.949	19.515	20.083	1.00	17.64

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ATOM	2167	CA	GLY	Α	334	55.123	20.340	18.903	1.00 16.89
ATOM	2168	C	GLY			55.205	19.663	17.548	1.00 17.61
MOTA	2169.	0	GLY			55.403	20.370	16.512	1.00 17.50
MOTA	2170	N	THR	Α	335	55.060	18.343	17.490	1.00 16.55
MOTA	2171	CA	THR	Δ	335	55.146	17.648	16.182	1.00 17.58
						53.802	17.260	15.557	1.00 16.83
MOTA	2172	C	THR						
ATOM	2173	0	THR	Α	335	53.761	16.408	14.618	1.00 17.71
ATOM	2174	CB	THR	Α	335	56.017	16.377	16.275	1.00 17.76
		OG1	THR			55.361	15.401	17.095	1.00 17.56
MOTA	2175				•				
MOTA	2176	CG2	THR	A	335	57.373	16.710	16.884	1.00 17.23
ATOM	2177	N	THR	Α	336	52.707	17.842	16.037	1.00 16.75
ATOM	2178	CA	THR	Δ	336	51.373	17.527	15.460	1.00 16.56
MOTA	2179 ·	C	THR			51.473	17.752	13.952	1.00 16.24
ATOM	2180	0	THR	Α	336	51.821	18.868	13.487	1.00 16.30
MOTA	2181	CB	THR	Α	336	50.267	18.437	16.030	1.00 17.05
ATOM	2182	OG1				50.181	18.255	17.451	1.00 17.15
MOTA	2183	CG2	THR			48.917	18.096	15.401	1.00 16.72
ATOM	2184	N	PRO	A	337	51.182	16.718	13.157	1.00 15.50
ATOM	2185	CA	PRO	Α	337	51.254	16.820	11.699	1.00 14.87
ATOM	2186	Ç	PRO			50.006	17.444	11.082	1.00 14.56
MOTA	2187	0	PRO			49.310	16.800	10.249	1.00 14.49
ATOM	2188	CB	PRO	Α	337	51.448	15.369	11.281	1.00 15.18
MOTA	2189	CG	PRO	A	337	50.520	14.657	12.238	1.00 16.05
	2190	CD	PRO			50.784	15.359	13.572	1.00 15.54
MOTA									
MOTA	2191	N	TRP			49.713	18.682	11.470	1.00 14.89
ATOM	2192	CA	TRP	Α	338	48.535	19.415	10.956	1.00 14.85
MOTA	2193	C	TRP	Δ	338	48.339	19.304	9.445	1.00 14.87
						47.194	19.048	8.966	1.00 17.13
MOTA	2194	0	TRP						
ATOM	2195	CB	TRP	А	338	48.639	20.899	11.313	1.00 13.77
ATOM	2196	CG	TRP	Α	338	48.784	21.176	12.767	1.00 15.11
ATOM	2197		TRP	Δ	338	49.897	21.652	13.411	1.00 14.78
								13.771	1.00 14.17
MOTA	2198	CD2	TRP			47.780	21.011		
MOTA	2199	NE1	TRP	A	338	49.641	21.794	14.756	1.00 14.64
ATOM	2200	CE2	TRP	Α	338 '	48.348	21.407	15.003	1.00 14.35
ATOM	2201	CE3	TRP			46.451	20.566	13.751	1.00 14.31
								16.202	1.00 14.86
MOTA	2202	CZ2	TRP			47.635	21.371		
MOTA	2203	CZ3	TRP	Α	338	45.744	20.530	14.945	1.00 16.02
ATOM	2204	CH2	TRP	A	338	46.339.	20.932	16.154	1.00 14.77
ATOM	2205	N	ASN	Α	339	49.414	19.486	8.682	1.00 13.22
			ASN			49.319	19.449	7.203	1.00 12.87
ATOM	2206	CA							
MOTA	2207	С	ASN			48.674	18.208	6.608	1.00 12.01
ATOM	2208	0	ASN	A	339	48.061	18.288	5.508	1.00 13.99
MOTA	2209	CB	ASN			50.699	19.649	6.552	1.00 12.61
			ASN			51.576	18.404	6.627	1.00 15.28
MOTA	2210	CG							
MOTA	2211		ASN				18.174	7.648	1.00 16.29
MOTA	2212	ND2	ASN	A	339	51.541	17.584	5.578	1.00 12.93
ATOM	2213	N	ILE			48.774	17.064	7.276	1.00 12.88
			ILE			48.171	15.831	6.698	1.00 12.98
ATOM	2214	CA							
MOTA	2215	C	ILE	Α	340	46.655	15.864	6.794	1.00 12.80
ATOM	2216	0	ILE	Α	340	45.944	15.237	5.959	1.00 12.80
MOTA	2217	СВ	ILE			48.667	14.545	7.400	1.00 14.79
								8.833	1.00 14.91
MOTA	2218	CG1				48.142	14.512		
ATOM	2219		ILE			50.194	14.483	7.372	1.00 12.38
ATOM	2220	CD1	ILE	Α	340	48.177	13.142	9.454	1.00 17.42
ATOM	2221	N	PHE			46.138	16.577	7.790	1.00 13.19
								7.972	1.00 13.87
MOTA	2222		PHE	A	J41	44.677	16.689		
MOTA	2223	С	PHE			44.143	17.741	7.006	1.00 13.37
ATOM	2224	0	PHE	Α	341	44.787	18.812	6.798	1.00 12.72
ATOM	2225	СВ	PHE			44.354	17.087	9.410	1.00 13.10
								10.429	1.00 13.55
MOTA	2226	CG	PHE				16.027		
MOTA	2227		PHE				14.960	10.654	1.00 13.48
MOTA	2228	CD2	PHE	Α	341	45.861	16.104	11.171	1.00 12.12

MOTA	2229	CE1	PHE	Α	341	44.115	13.984	11.607	1.00 13.44
ATOM ·	2230	CE2	PHE	A	341	46.172	15.136	12.127	1.00 14.31
MOTA	2231	CZ			341	45.298	14.074	12.346	1.00 13.92
ATOM	2232	N			342	42.975	17.484	6.402	1.00 12.78
MOTA	2233	CA	PRO	Α	342	42.357	18.413	5.448	1.00 12.17
MOTA	2234	С	PRO	Α	342	41.565	19.544	6.100	1.00 12.90
ATOM	2235	0			342	41.168	19.465	7.309	1.00 12.52
MOTA	2236	СВ			342	41.447	17.502	4.638	1.00 10.18
MOTA	2237	CG			342	40.920	16.570	5.714	1.00 11.48
ATOM	2238	CD	PRO	A	342	42.180	16.244	6.523	1.00 12.10
MOTA	2239	N	VAL	Α	343	41.342	20.609	5.342	1.00 12.27
MOTA	2240	CA	VAL	Α	343	40.528	21.712	5.851	1.00 10.51
ATOM	2241	C			343	39.101	21.281	5.521	1.00 12.41
ATOM	2242	Ö			343	38.878	20.401	4.632	1.00 10.45
MOTA	2243	CB			343	40.838	23.054	5.143	1.00 10.23
MOTA	2244	CG1	VAL	Α	343	42.247	23.507	5.488	1.00 8.58
ATOM	2245	CG2	VAL	Α	343	40.672	22.914	3.636	1.00 8.08
ATOM	2246	N	ILE	Α	344	38.132	21.848	6.224	1.00 13.49
ATOM	2247	CA			344	36.725	21.507		1.00 13.17
ATOM	2248	C			344	35.989	22.789	5.664	1.00 13.33
MOTA	2249	0			344	36.067	23.795	6.427	1.00 13.12
MOTA	2250	CB			344	36.099	20.859	7.246	1.00 14.77
MOTA	2251	CG1	ILE	Α	344	36.776	19.512	7.517	1.00 14.50
ATOM	2252	CG2	ILE	Α	344	34.585	20.702	7.060	1.00 13.14
ATOM	2253	CD1	ILE	Α	344	36.374	18.875	8.825	1.00 17.73
ATOM	2254	N			345	35.292	22.794	4.537	1.00 12.41
ATOM	2255	CA			345	34.547	23.982	4.136	1.00 13.41
ATOM	2256	C	SER			33.051	23.723	4.172	1.00 14.94
MOTA	2257	0	SER			32.555	22.641	3.721	1.00 14.55
MOTA	2258	CB	SER	А	345	34.967	24.430	2.728	1.00 14.23
MOTA	2259	OG	SER	Α	345	36.329	24.834	2.703	1.00 13.57
ATOM	2260	N	LEU	A	346	32.320	24.682	4.725	1.00 13.42
ATOM	2261	CA	LEU			30.859	24.594	4.796	1.00 14.08
ATOM	2262	C	LEU			30.320	25.772	4.003	1.00 13.86
ATOM	2263	0	LEU			30.681	26.956	4.286	1.00 13.52
ATOM	2264	CB	LEU			30.383	24.674	6.252	1.00 15.83
MOTA	2265	CG	LEU			30.239	23.372	7.051	1.00 17.74
MOTA	2266	CD1	LEU	Α	346	31.455	22.492	6.875	1.00 18.92
MOTA	2267	CD2	LEU	Α	346	30.028	23.711	8.521	1.00 19.69
MOTA	2268	N	TYR	Α	347	29.496	25.485	3.000	1.00 13.48
MOTA	2269	CA	TYR			28.894	26.543	2.176	1.00 13.76
MOTA	2270	C	TYR			27.525	26.864	2.745	1.00 14.58
ATOM	2271	0	TYR			26.676			1.00 13.16
MOTA	2272	CB	TYR			28.757		0.716	1.00 14.82
ATOM	2273	CG	TYR			30.066	26.051	-0.034	1.00 15.10
MOTA	2274	CD1	TYR	A	347	31.022	25.074	0.252	1.00 13.97
ATOM	2275	CD2	TYR	Α	347	30.349	26.977	-1.038	1.00 13.98
ATOM	2276	CE1	TYR	Α	347	32.228	25.018	-0.447	1.00 14.47
ATOM	2277				347	31.556	26.930	-1.746	1.00 15.69
							25.949		
MOTA	2278	CZ	TYR			32.487		-1.445	1.00 15.09
MOTA	2279	OH	TYR			33.672	25.895	-2.141	1.00 16.72
ATOM	2280	N	LEU			27.288	28.145	2.971	1.00 13.86
MOTA	2281	CA	LEU	Α	348	26.018	28.593	3.545	1.00 16.70
MOTA	2282	C	LEU	Α	348	25.246	29.445	2.559	1.00 17.37
ATOM	2283	Ō	LEU				30.183	1.722	1.00 16.05
ATOM	2284	СВ	LEU			26.292	29.401	4.814	1.00 15.57
								5.908	
MOTA	2285	CG	LEU			27.019	28.620		1.00 17.10
ATOM	2286		LEU				29.565	6.985	1.00 15.71
MOTA	2287		LEU				27.580	6.495	1.00 16.92
MOTA	2288	N	MET				29.352	2.617	1.00 19.68
MOTA	2289	CA	MET	Α	349	23.073	30.167	1.734	1.00 22.78
MOTA	2290	С	MET	Α	349	23.384	31.629	2.024	1.00 22.03

ATOM 2291 O MET A 349 21.594 32.049 3.222 1.00 20.70 ATOM 2292 CB MET A 349 21.594 29.897 2.008 1.00 25.40 ATOM 2293 CG MET A 349 21.594 29.897 2.008 1.00 25.40 ATOM 2295 CF MET A 349 19.139 28.933 1.272 1.00 37.43 ATOM 2295 N GLY A 350 23.573 32.414 0.972 1.00 23.73 ATOM 2297 CA GLY A 350 23.573 33.824 1.167 1.00 32.50 ATOM 2298 C GLY A 350 22.565 34.612 1.280 1.00 23.50 ATOM 2299 O GLY A 350 22.565 34.612 1.280 1.00 23.50 ATOM 2300 N GLU A 351 22.662 35.899 1.591 1.00 27.25 ATOM 2301 CA GLU A 351 21.448 36.734 1.698 1.00 23.13 ATOM 2301 C GLU A 351 21.448 36.734 1.698 1.00 32.00 ATOM 2302 C GLU A 351 21.474 38.081 2.340 1.00 32.31 ATOM 2303 O GLU A 351 19.620 37.065 0.125 1.00 34.42 ATOM 2304 CB GLU A 351 22.012 37.965 0.125 1.00 34.92 ATOM 2305 CG GLU A 351 22.012 37.965 0.125 1.00 34.92 ATOM 2306 CD GLU A 351 22.012 37.965 0.125 1.00 34.92 ATOM 2308 OEZ GLU A 351 22.012 37.965 0.254 1.00 32.31 ATOM 2309 N VAL A 352 21.753 37.007 -0.684 1.00 36.55 ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.29 ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.29 ATOM 2311 C VAL A 352 21.753 37.007 -0.684 1.00 36.29 ATOM 2312 O VAL A 352 21.753 37.007 -0.684 1.00 36.29 ATOM 2313 C VAL A 352 21.699 37.892 -4.392 1.00 36.29 ATOM 2315 CG VAL A 352 21.999 37.892 -4.266 1.00 39.68 ATOM 2315 CG VAL A 352 21.999 37.892 -4.266 1.00 39.68 ATOM 2315 CG VAL A 352 21.999 37.892 -4.266 1.00 39.68 ATOM 2316 N THR A 353 19.806 35.7767 -2.999 1.00 40.47 ATOM 2317 CA THR A 353 19.806 35.7767 -2.999 1.00 40.397 ATOM 2310 CA VAL A 352 21.999 37.892 -4.261 1.00 36.39 ATOM 2310 CA VAL A 352 21.999 37.892 -4.262 1.00 36.31 ATOM 2310 CA VAL A 352 21.999 37.892 -4.299 1.00 40.47 ATOM 2311 C VAL A 352 21.999 37.892 -4.299 1.00 40.47 ATOM 2312 CO THR A 353 19.806 35.7767 -2.999 1.00 40.40 ATOM 2320 CB THR A 353 19.806 35.7767 -2.999 1.00 40.40 ATOM 2321 CG THR A 353 19.306 31.476 -3.511 1.00 45.29 ATOM 2321 CG THR A 353 19.306 31.476 -3.511 1.00 45.64 ATOM 2322 CG SAN A 354 20.494 32.994 -4.194 1.00 45.64 ATOM 2323 CG SAN A 354 20.494 32.999											
ATOM 2292 CB MET A 349 20.931 29.897 2.008 1.00 25.40 ATOM 2293 CG MET A 349 20.931 28.954 1.012 1.00 31.18 ATOM 2295 CB MET A 349 19.139 28.833 1.272 1.00 37.43 ATOM 2295 CB MET A 349 19.139 28.833 1.272 1.00 37.43 ATOM 2295 CB MET A 350 23.573 30.583 1.318 1.00 22.516 ATOM 2297 CA GLY A 350 23.573 31.824 1.167 1.00 23.50 ATOM 2299 C GLY A 350 22.565 34.612 1.280 1.00 24.26 ATOM 2299 C GLY A 350 22.565 34.612 1.280 1.00 24.26 ATOM 2300 N GLU A 351 22.662 38.699 1.091 1.00 23.50 ATOM 2301 CA GLU A 351 22.662 35.899 1.591 1.00 27.25 ATOM 2301 CA GLU A 351 20.870 36.948 0.306 1.00 33.92 ATOM 2301 CA GLU A 351 20.870 36.948 0.306 1.00 32.90 ATOM 2302 C GLU A 351 20.870 36.948 0.306 1.00 32.90 ATOM 2302 C GLU A 351 20.870 37.065 0.125 1.00 34.42 ATOM 2305 CG GLU A 351 22.012 37.966 3.831 1.00 32.91 ATOM 2305 CG GLU A 351 22.012 37.966 3.831 1.00 32.91 ATOM 2305 CG GLU A 351 22.012 37.966 3.831 1.00 32.91 ATOM 2305 CG GLU A 351 22.012 37.996 3.831 1.00 32.91 ATOM 2305 CG GLU A 351 22.012 37.996 3.831 1.00 32.91 ATOM 2305 CG GLU A 351 22.012 37.996 3.831 1.00 35.55 ATOM 2307 CEI GLU A 351 22.819 40.187 4.293 1.00 36.64 ATOM 2308 OE2 GLU A 351 22.819 40.187 4.293 1.00 36.64 ATOM 2300 CA VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2310 CA VAL A 352 21.327 37.811 -2.082 1.00 38.72 ATOM 2311 C VAL A 352 22.456 37.767 -2.939 1.00 38.31 ATOM 2316 CG GLU A 351 22.21 3.996 33.4799 -2.629 1.00 40.47 ATOM 2310 CA VAL A 352 22.456 37.767 -2.939 1.00 38.31 ATOM 2315 CG VAL A 352 22.456 37.767 -2.939 1.00 38.31 ATOM 2315 CG VAL A 352 22.496 39.133 -2.491 1.00 37.93 ATOM 2315 CG VAL A 352 22.496 39.133 -2.491 1.00 37.93 ATOM 2315 CG VAL A 352 22.496 39.133 -2.491 1.00 37.93 ATOM 2315 CG VAL A 352 22.496 39.133 -2.491 1.00 37.93 ATOM 2315 CG VAL A 352 22.496 39.133 -2.491 1.00 37.93 ATOM 2315 CG VAL A 352 22.496 39.133 -2.491 1.00 37.93 ATOM 2315 CG VAL A 352 22.496 39.136 -2.461 1.00 32.50 ATOM 2315 CG VAL A 352 22.496	ATOM	2291	0	MET .	A 349	23.	478 3	32.049	3.222	1.00	20.70
ATOM   2293   CG   MET   A 349   20,931   28,954   1.012   1.00   31,18   ATOM   2294   SD   MET   A 349   19,139   28,833   1.312   1.00   37,43   ATOM   2295   CE   MET   A 349   18,697   30,583   1.318   1.00   32,73   ATOM   2297   CA   GLV   A 350   23,573   32,414   0.972   1.00   23,50   ATOM   2298   C   GLV   A 350   23,573   33,824   1.167   1.00   23,50   ATOM   2298   C   GLV   A 350   22,565   34,612   1.280   1.00   23,13   ATOM   2299   O   GLV   A 350   22,565   34,612   1.280   1.00   23,13   ATOM   2300   N   GLU   A 351   22,662   35,899   1.591   1.00   23,13   ATOM   2300   C   GLU   A 351   21,448   36,734   1.698   1.00   32,03   ATOM   2302   C   GLU   A 351   21,448   36,734   1.698   1.00   32,03   ATOM   2302   C   GLU   A 351   21,474   38,081   2.340   1.00   32,31   ATOM   2303   O   GLU   A 351   19,620   37,066   0.125   1.00   34,42   ATOM   2304   CB   GLU   A 351   21,916   39,346   4.693   1.00   32,31   ATOM   2305   CG   GLU   A 351   22,819   40,187   4.293   1.00   36,54   ATOM   2306   CD   GLU   A 351   22,819   40,187   4.293   1.00   36,64   ATOM   2309   N   VAL   A 352   21,755   37,007   -0.684   1.00   36,78   ATOM   2300   CD   GLU   A 351   22,819   40,187   4.293   1.00   36,64   ATOM   2310   CA   VAL   A 352   21,755   37,007   -0.684   1.00   36,98   ATOM   2310   CA   VAL   A 352   21,755   37,007   -0.684   1.00   36,98   ATOM   2310   CA   VAL   A 352   21,357   37,007   -0.684   1.00   36,98   ATOM   2312   CO   VAL   A 352   21,999   37,892   -4.436   1.00   36,98   ATOM   2312   CO   VAL   A 352   21,999   37,892   -4.436   1.00   36,98   ATOM   2312   CO   VAL   A 352   21,999   37,892   -4.436   1.00   36,98   ATOM   2312   CO   VAL   A 352   21,999   37,892   -4.436   1.00   36,98   ATOM   2312   CO   VAL   A 352   21,999   37,892   -4.436   1.00   36,98   ATOM   2312   CO   VAL   A 352   21,999   37,892   -4.436   1.00   36,98   ATOM   2312   CO   VAL   A 352   21,999   37,892   -4.436   1.00   36,98   ATOM   2313   CO   VAL   A 352   21,999   37			CB			21.	594 2	9.897	2.008	1.00	25.40
ATOM 2295 CB MET A 349 19 139 28 833 1.272 1.00 37.43 ATOM 2295 CB MET A 349 18.697 30.583 1.318 1.00 32.73 ATOM 2296 N GLY A 350 23.573 32.414 0.972 1.00 20.81 ATOM 2298 C GLY A 350 23.573 32.414 0.972 1.00 20.81 ATOM 2298 C GLY A 350 22.565 34.612 1.280 1.00 24.26 ATOM 2299 C GLY A 350 22.565 34.612 1.280 1.00 24.26 ATOM 2300 N GLU A 351 22.662 35.899 1.591 1.00 27.25 ATOM 2301 CA GLU A 351 21.448 36.734 1.698 1.00 32.00 ATOM 2302 C GLU A 351 21.448 36.734 1.698 1.00 32.00 ATOM 2303 C GLU A 351 21.448 36.734 1.698 1.00 33.92 ATOM 2303 C GLU A 351 19.620 37.065 0.125 1.00 34.42 ATOM 2304 CB GLU A 351 19.620 37.065 0.125 1.00 34.42 ATOM 2305 CG GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2306 CD GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2308 CC GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2308 CC GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2308 CC GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2308 CC GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2308 CC GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2308 CC GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2301 CA VAL A 352 21.375 37.007 -0.684 1.00 36.64 ATOM 2301 CA VAL A 352 21.997 39.567 5.233 1.00 36.98 ATOM 2310 CA VAL A 352 21.393 37.007 -0.684 1.00 36.98 ATOM 2311 C VAL A 352 21.393 37.007 -0.684 1.00 36.98 ATOM 2311 C VAL A 352 21.393 37.767 -2.939 1.00 38.31 ATOM 2315 CGV VAL A 352 21.999 37.892 -2.426 1.00 38.33 ATOM 2316 N THR A 353 19.300 34.476 -3.882 1.00 38.33 ATOM 2316 N THR A 353 19.300 34.476 -3.882 1.00 38.33 ATOM 2316 N THR A 353 19.300 34.476 -3.882 1.00 38.33 ATOM 2316 N THR A 353 19.300 34.476 -3.882 1.00 38.33 ATOM 2317 CA THR A 353 19.300 34.476 -3.882 1.00 34.98 ATOM 2320 CB THR A 353 19.300 34.476 -3.882 1.00 43.98 ATOM 2321 CG THR A 353 19.300 34.476 -3.882 1.00 43.18 ATOM 2321 CG THR A 353 19.300 34.476 -3.882 1.00 34.98 ATOM 2322 CG ANN A 354 22.641 32.166 -5.681 1.00 47.73 ATOM 2323 C G SNN A 354 22.499 34.699 -2.699 1.00 40.77 3.700 2325 C G SNN A 354 22.647 37.32 3.042 -4.877 1.00 45.63 ATOM 2332 C G SNN A 355 22.497 34.679											
ATOM 2295 CE MET A 3499 18.697 30.583 1.318 1.00 32.73 ATOM 2297 CA GLY A 350 23.573 32.414 0.972 1.00 20.81 ATOM 2298 C GLY A 350 23.573 32.414 1.167 1.00 23.50 ATOM 2298 C GLY A 350 22.565 34.612 1.280 1.00 24.26 ATOM 2299 O GLY A 350 22.565 34.612 1.280 1.00 24.26 ATOM 2301 CA GLU A 351 22.662 35.899 1.591 1.00 23.13 ATOM 2301 CA GLU A 351 22.662 35.899 1.591 1.00 27.25 ATOM 2302 C GLU A 351 20.870 36.948 0.306 1.00 32.00 ATOM 2303 O GLU A 351 20.870 36.948 0.306 1.00 34.42 ATOM 2303 O GLU A 351 20.870 36.948 0.306 1.00 34.92 ATOM 2305 CG GLU A 351 21.448 36.734 1.698 1.00 32.00 ATOM 2305 CG GLU A 351 22.7174 38.081 2.340 1.00 32.42 ATOM 2305 CG GLU A 351 22.7174 38.081 2.340 1.00 32.37 ATOM 2305 CG GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2306 CD GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2307 OEI GLU A 351 22.919 40.187 4.293 1.00 36.64 ATOM 2308 OE2 GLU A 351 22.917 39.567 5.233 1.00 36.298 ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2311 C VAL A 352 21.327 37.181 -2.082 1.00 36.72 ATOM 2312 O VAL A 352 21.999 37.892 -2.629 1.00 38.37 ATOM 2312 C VAL A 352 22.456 37.767 -2.939 1.00 38.37 ATOM 2313 CB VAL A 352 22.456 37.767 -2.939 1.00 38.37 ATOM 2314 CGI VAL A 352 22.499 37.892 -4.382 1.00 38.33 ATOM 2315 CG VAL A 352 22.499 37.892 -4.382 1.00 38.33 ATOM 2316 C TRIR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2316 N THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2316 C TRIR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2317 CA THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2319 O THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2321 OGI THR A 353 19.806 39.123 -4.871 1.00 37.92 ATOM 2322 CG THR A 353 19.806 35.747 -3.314 1.00 42.20 ATOM 2323 N ASN A 354 22.641 32.166 39.123 -4.871 1.00 43.93 ATOM 2320 CB THR A 353 19.806 35.747 -3.314 1.00 42.20 ATOM 2321 OGI THR A 353 19.806 35.747 -3.314 1.00 42.20 ATOM 2322 CG ASN A 354 22.641 32.165 -5.611 1.00 41.22 ATOM 2323 CG GLN A 355 22.999 32.627 -4.899 1.00 42.00 4.004 3.004 3.004 3.004		-									
ATOM 2296 N GLY A 350											
ATOM 2299 C GLY A 350	MOTA	2295	CE	MET .	A 349						
ATOM 2298 C GLY A 350	ATOM	2296	N	GLY :	A 350	23.	573 3	32.414	0.972	1.00	20.81
ATOM 2298 C GLY A 350	ATOM	2297	CA ·	GLY .	A 350	23.	857 3	3.824	1.167	1.00	23.50
ATOM 2309 O GLY A 350						22.	565 3	4.612		1.00	24.26
ATOM 2300 N GLU A 351											
ATOM 2301 CA GLU A 351 21.448 36.734 1.698 1.00 32.00 ATOM 2302 C GLU A 351 20.870 36.948 0.306 1.00 33.92 ATOM 2303 O GLU A 351 19.620 37.065 0.125 1.00 34.42 ATOM 2304 CB GLU A 351 21.774 38.081 2.340 1.00 32.31 ATOM 2306 CD GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2306 CD GLU A 351 22.012 37.996 3.831 1.00 34.52 ATOM 2307 OEI GLU A 351 22.819 40.187 4.293 1.00 35.55 ATOM 2307 OEI GLU A 351 22.819 40.187 4.293 1.00 36.64 ATOM 2309 N VAL A 352 22.819 40.187 4.293 1.00 36.64 ATOM 2309 N VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2310 CA VAL A 352 21.327 37.181 -2.082 1.00 36.98 ATOM 2311 C VAL A 352 21.693 44.799 -2.629 1.00 40.47 ATOM 2312 O VAL A 352 22.694 35.809 -2.629 1.00 40.47 ATOM 2313 CB VAL A 352 22.456 37.767 -2.939 1.00 38.31 ATOM 2314 CCI VAL A 352 22.456 37.767 -2.939 1.00 38.31 ATOM 2315 CAZ TAL A 352 22.456 37.767 -2.939 1.00 38.33 ATOM 2315 CAZ TAL A 352 22.456 37.767 -2.939 1.00 38.33 ATOM 2316 N THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2316 N THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2316 CAZ TAL A 352 22.866 39.123 -2.391 1.00 37.08 ATOM 2317 CA THR A 353 19.806 35.747 -3.314 1.00 43.18 ATOM 2319 O THR A 353 19.300 34.476 -3.882 1.00 43.97 ATOM 2318 C THR A 353 19.300 34.476 -3.882 1.00 43.97 ATOM 2318 C THR A 353 19.300 34.476 -3.882 1.00 43.93 ATOM 2318 C THR A 353 17.992 34.596 -5.688 1.00 43.93 ATOM 2322 CG2 THR A 353 16.849 34.988 -3.551 1.00 43.18 ATOM 2322 CG2 THR A 353 17.992 34.576 -4.5878 1.00 45.25 ATOM 2322 CG2 THR A 353 16.849 34.988 -3.551 1.00 43.18 ATOM 2322 CG2 THR A 353 17.992 34.6767 -4.879 1.00 43.18 ATOM 2322 CG2 THR A 353 17.992 34.6767 -4.879 1.00 43.18 ATOM 2323 N ASN A 354 20.307 32.507 -4.839 1.00 43.04 ATOM 2324 CA ASN A 354 20.307 32.507 -4.839 1.00 43.04 ATOM 2325 CG ASN A 354 20.307 32.507 -4.839 1.00 43.04 ATOM 2326 CG ASN A 354 20.307 32.507 -4.839 1.00 43.04 ATOM 2327 CB ASN A 354 20.307 32.507 -4.839 1.00 43.04 ATOM 2328 CG ASN A 354 20.307 32.507 -4.839 1.00 43.04 ATOM 2331 N GLN A 355 22.999 32.621 -4.419 1.00 37.62 ATOM 2334 O GLN A 35											
ATOM 2302 C GLU A 351 19.620 37.066 0.306 1.00 33.92 ATOM 2303 O GLU A 351 19.620 37.066 0.125 1.00 34.42 ATOM 2304 CB GLU A 351 21.774 38.081 2.340 1.00 32.31 ATOM 2305 CG GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2306 CD GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2307 OEI GLU A 351 22.819 40.187 4.293 1.00 36.64 ATOM 2308 OEZ GLU A 351 20.927 39.567 5.233 1.00 36.64 ATOM 2308 OEZ GLU A 351 20.927 39.567 5.233 1.00 36.98 ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2310 CA VAL A 352 21.327 37.181 -2.082 1.00 38.72 ATOM 2311 C VAL A 352 21.327 37.181 -2.082 1.00 38.72 ATOM 2312 O VAL A 352 22.456 37.767 -2.939 1.00 39.68 ATOM 2313 CB VAL A 352 22.456 37.767 -2.939 1.00 39.68 ATOM 2313 CC VAL A 352 22.456 37.767 -2.939 1.00 39.68 ATOM 2314 CGI VAL A 352 22.9456 37.767 -2.939 1.00 38.31 ATOM 2315 CGZ VAL A 352 22.866 39.123 -2.391 1.00 37.93 ATOM 2315 CGZ VAL A 353 19.806 35.747 -3.314 1.00 42.37 ATOM 2315 CGZ VAL A 353 19.806 35.747 -3.314 1.00 42.37 ATOM 2317 CA THR A 353 19.806 35.747 -3.314 1.00 42.37 ATOM 2318 C THR A 353 19.806 35.747 -3.314 1.00 42.37 ATOM 2319 O THR A 353 19.806 35.747 -3.314 1.00 42.27 ATOM 2321 OGI THR A 353 19.300 34.476 -3.882 1.00 38.18 ATOM 2321 OGI THR A 353 19.300 34.676 -5.688 1.00 42.63 ATOM 2322 CGZ THR A 353 16.808 35.743 -3.832 -4.877 1.00 45.29 ATOM 2322 CGZ THR A 353 16.808 37.992 34.672 -4.578 1.00 45.29 ATOM 2322 CGZ THR A 353 16.808 37.993 38.38 -4.877 1.00 45.29 ATOM 2322 CGZ THR A 353 16.808 37.993 38.38 -4.877 1.00 45.23 ATOM 2323 N ASN A 354 22.641 32.166 -5.611 1.00 46.31 ATOM 2323 N ASN A 354 22.641 32.166 -5.611 1.00 47.73 ATOM 2323 CG ASN A 354 22.473 32.507 -4.839 1.00 42.20 ATOM 2323 CG GAN A 355 22.475 32.475 -2.764 1.00 43.04 ATOM 2323 CG GAN A 355 22.475 32.863 2.868 3.8797 -1.00 23.68 ATOM 2333 CG GLN A 355 24.4737 32.2475 -2.764 1.00 47.73 ATOM 2336 CG GLN A 355 24.4737 32.2475 -2.764 1.00 47.73 ATOM 2337 CD GLN A 355 24.4737 32.2475 -2.764 1.00 47.73 ATOM 2336 CG GLN A 355 25.834 35.089 -3.797 1.00 29.36 ATOM 2337 CD GLN A 355 25.839											
ATOM 2303 O GLU A 351 19.620 37.066 0.125 1.00 34.42 ATOM 2305 CG GLU A 351 21.774 38.081 2.340 1.00 32.31 ATOM 2305 CG GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2306 CD GLU A 351 22.819 40.187 4.293 1.00 36.55 ATOM 2307 OEI GLU A 351 22.819 40.187 4.293 1.00 36.55 ATOM 2308 OEZ GLU A 351 22.819 40.187 4.293 1.00 36.55 ATOM 2309 N VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2311 C VAL A 352 21.327 37.181 -2.082 1.00 36.98 ATOM 2312 O VAL A 352 21.689 34.799 -2.629 1.00 40.47 ATOM 2313 CB VAL A 352 22.456 37.767 -2.939 1.00 38.31 ATOM 2314 CCI VAL A 352 22.866 39.123 -2.391 1.00 38.31 ATOM 2315 CGZ VAL A 352 22.866 39.123 -2.391 1.00 38.31 ATOM 2316 N THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2317 CA THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2318 C THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2319 O THR A 353 20.941 34.536 -5.688 1.00 42.65 ATOM 2320 CB THR A 353 17.929 34.672 -4.578 1.00 43.97 ATOM 2320 CB THR A 353 18.018 35.556 3.688 1.00 42.65 ATOM 2321 CGI THR A 353 18.018 35.556 1.00 46.63 ATOM 2321 CGI THR A 353 18.018 35.556 1.00 46.63 ATOM 2322 CGZ THR A 353 18.018 35.551 1.00 42.33 ATOM 2322 CGZ THR A 353 18.018 35.747 -3.314 1.00 42.33 ATOM 2322 CGZ THR A 353 18.018 35.747 -3.314 1.00 42.33 ATOM 2322 CGZ THR A 353 18.018 35.747 -4.878 1.00 43.39 ATOM 2322 CGZ GASN A 354 21.183 31.741 -5.742 1.00 42.30 ATOM 2322 CGZ GASN A 354 21.183 31.741 -5.742 1.00 42.20 ATOM 2323 CG ASN A 354 21.183 31.741 -5.742 1.00 43.39 ATOM 2324 CA ASN A 354 21.183 31.741 -5.742 1.00 42.20 ATOM 2325 C ASN A 354 21.183 31.741 -5.742 1.00 45.64 ATOM 2325 C ASN A 354 21.183 31.741 -5.742 1.00 45.64 ATOM 2328 C G GLN A 355 22.999 32.621 -4.419 1.00 37.65 ATOM 2332 C G GLN A 355 22.999 32.621 -4.419 1.00 37.65 ATOM 2333 C G GLN A 355 22.999 32.621 -4.419 1.00 37.0	MOTA	2301									
ATOM 2305 CB GLU A 351	MOTA	2302	С	GLU :	A 351	20.					
ATOM 2306 CG GLU A 351 22.012 37.996 3.831 1.00 34.92 ATOM 2306 CD GLU A 351 21.916 39.346 4.503 1.00 35.55 ATOM 2307 OEI GLU A 351 22.919 40.187 4.293 1.00 36.64 ATOM 2308 OE2 GLU A 351 20.927 39.567 5.233 1.00 36.98 ATOM 2310 CA VAL A 352 21.327 37.181 -2.082 1.00 38.72 ATOM 2311 C VAL A 352 21.327 37.181 -2.082 1.00 38.72 ATOM 2312 O VAL A 352 21.327 37.181 -2.082 1.00 38.72 ATOM 2312 O VAL A 352 21.689 34.799 -2.426 1.00 39.68 ATOM 2313 CB VAL A 352 22.456 37.767 -2.939 1.00 39.68 ATOM 2314 CGI VAL A 352 22.456 37.767 -2.939 1.00 38.31 ATOM 2315 CG2 VAL A 352 22.456 37.767 -2.939 1.00 38.31 ATOM 2316 N THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2316 N THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2318 C THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2318 C THR A 353 19.806 35.747 -3.382 1.00 42.394 ATOM 2319 O THR A 353 19.806 35.747 -3.882 1.00 42.394 ATOM 2319 O THR A 353 19.806 35.747 -3.882 1.00 42.63 ATOM 2321 OGI THR A 353 19.300 34.476 -3.882 1.00 42.63 ATOM 2322 CG2 THR A 353 17.929 34.672 -4.578 1.00 42.52 ATOM 2323 N ASN A 354 20.941 34.536 -5.688 1.00 42.52 ATOM 2322 CG2 THR A 353 16.849 34.989 -3.551 1.00 46.31 ATOM 2323 N ASN A 354 20.497 34.989 -3.551 1.00 46.33 ATOM 2323 N ASN A 354 20.497 34.989 -3.551 1.00 46.33 ATOM 2325 C ASN A 354 20.498 34.989 -3.551 1.00 46.34 ATOM 2327 CB ASN A 354 20.698 31.887 -7.187 1.00 43.39 ATOM 2328 CG ASN A 354 20.698 31.887 -7.187 1.00 43.04 ATOM 2329 ODI ASN A 354 20.698 31.887 -7.187 1.00 43.04 ATOM 2329 ODI ASN A 355 24.4371 30.059 -6.584 1.00 47.44 ATOM 2330 ND2 ASN A 354 19.467 31.065 -7.187 1.00 49.64 ATOM 2331 N GLN A 355 24.4371 30.042 -4.128 1.00 34.85 ATOM 2332 C GLN A 355 24.459 34.580 -4.105 1.00 34.85 ATOM 2333 N C GLN A 355 24.477 32.475 -2.764 1.00 32.57 ATOM 2334 O GLN A 355 25.586 37.171 -4.992 1.00 49.74 ATOM 2339 ND2 ASN A 354 28.459 34.589 -3.797 1.00 39.05 ATOM 2331 N GLN A 355 24.459 34.580 -4.105 1.00 34.85 ATOM 2333 C GLN A 355 25.586 37.171 -4.992 1.00 40.57 ATOM 2334 O GLN A 355 25.586 37.171 -4.992 1.00 40.57 ATOM 2334 O SER A	MOTA	2303	0	GLU .	A 351	19.	620 3	7.066	0.125	1.00	34.42
ATOM 2305 CG GUU A 351	ATOM	2304	CB	GLU 2	A 351	21.	774 3	8.081	2.340	1.00	32.31
ATOM 2306 CD GLU A 351						22.	012 3	7.996	3.831	1.00	34.92
ATOM 2307 OE1 GLU A 351											
ATOM 2309 N VAL A 351											
ATOM 2310 CA VAL A 352 21.753 37.007 -0.684 1.00 36.98 ATOM 2310 CA VAL A 352 21.327 37.181 -2.082 1.00 40.47 ATOM 2311 C VAL A 352 21.327 37.181 -2.082 1.00 40.47 ATOM 2312 C VAL A 352 22.668 34.799 -2.426 1.00 39.68 ATOM 2313 CB VAL A 352 22.456 37.767 -2.939 1.00 38.33 ATOM 2314 CGI VAL A 352 22.456 37.767 -2.939 1.00 38.33 ATOM 2315 CG2 VAL A 352 22.866 39.123 -2.391 1.00 38.33 ATOM 2316 N THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2317 CA THR A 353 19.806 35.747 -3.314 1.00 43.97 ATOM 2317 CA THR A 353 20.254 33.832 -4.877 1.00 43.18 ATOM 2319 O THR A 353 20.941 34.536 -5.688 1.00 42.30 ATOM 2310 CG THR A 353 18.018 35.743 -5.526 1.00 45.29 ATOM 2320 CB THR A 353 18.018 35.743 -5.526 1.00 45.29 ATOM 2322 CG2 THR A 353 16.849 34.988 -3.551 1.00 45.29 ATOM 2323 N ASN A 354 20.307 32.507 -4.839 1.00 42.20 ATOM 2323 N ASN A 354 22.641 32.166 -5.611 1.00 42.20 ATOM 2325 C ASN A 354 22.641 32.166 -5.611 1.00 43.04 ATOM 2322 CB ASN A 354 22.641 32.166 -5.611 1.00 43.04 ATOM 2322 CB ASN A 354 22.641 32.166 -5.611 1.00 43.04 ATOM 2322 CB ASN A 354 22.641 32.166 -5.611 1.00 43.04 ATOM 2322 CB ASN A 354 22.641 32.166 -5.611 1.00 43.04 ATOM 2322 CB ASN A 354 22.641 32.166 -5.611 1.00 47.73 ATOM 2323 N CB ASN A 354 22.641 32.166 -5.611 1.00 47.73 ATOM 2329 ODI ASN A 354 19.467 31.036 -7.474 1.00 47.64 ATOM 2329 ODI ASN A 354 19.467 31.036 -7.474 1.00 47.73 ATOM 2331 N GLN A 355 22.999 32.621 -4.419 1.00 37.62 ATOM 2332 CG GLN A 355 22.999 32.621 -4.419 1.00 37.63 ATOM 2333 C GLN A 355 22.999 32.621 -4.419 1.00 37.63 ATOM 2334 C GLN A 355 22.999 32.621 -4.419 1.00 37.63 ATOM 2334 C GLN A 355 22.999 32.621 -4.419 1.00 37.63 ATOM 2334 C GLN A 355 22.999 32.621 -4.419 1.00 37.63 ATOM 2334 C GLN A 355 24.773 32.475 -2.764 1.00 39.68 ATOM 2334 C GLN A 355 24.737 32.475 -2.764 1.00 39.68 ATOM 2334 C GLN A 355 24.737 32.475 -2.764 1.00 39.68 ATOM 2334 C GLN A 355 24.633 3.999 -3.991 1.00 39.68 ATOM 2334 C GLN A 355 25.989 32.911 -2.597 1.00 29.56 ATOM 2340 C GLN A 355 25.989 32.911 -2.597 1.00 29.56 ATOM 2340 C GLN A 355 2											
ATOM 2311 C VAL A 352											
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ATOM 2313 CB VAL A 352	MOTA	2311	С	VAL .	A 352	20.	944 3	5.809	-2.629		
ATOM 2314 CGI VAL A 352	MOTA	2312	0	VAL .	A 352	21.	689 3	4.799	-2.426	1.00	39.68
ATOM 2314 CG1 VAL A 352 21.999 37.892 -4.382 1.00 38.33 ATOM 2315 CG2 VAL A 352 22.866 39.123 -2.391 1.00 37.93 ATOM 2316 N THR A 353 19.806 35.747 -3.314 1.00 42.33 ATOM 2317 CA THR A 353 19.806 35.747 -3.314 1.00 43.97 ATOM 2318 C THR A 353 20.254 33.832 -4.877 1.00 43.18 ATOM 2319 O THR A 353 20.254 33.832 -4.877 1.00 43.18 ATOM 2320 CB THR A 353 17.929 34.672 -4.578 1.00 45.29 ATOM 2321 OG1 THR A 353 18.018 35.743 -5.526 1.00 46.63 ATOM 2322 CG2 THR A 353 18.018 35.743 -5.526 1.00 46.63 ATOM 2323 N ASNA 354 20.307 32.507 -4.839 1.00 42.20 ATOM 2324 CA ASNA 354 20.307 32.507 -4.839 1.00 42.20 ATOM 2325 C ASNA 354 22.641 32.166 -5.611 1.00 43.39 ATOM 2325 C ASNA 354 22.641 32.166 -5.611 1.00 43.04 ATOM 2327 CB ASNA 354 20.698 31.887 -7.187 1.00 45.64 ATOM 2327 CB ASNA 354 20.698 31.887 -7.187 1.00 45.64 ATOM 2329 OD1 ASNA 354 19.467 31.036 -7.474 1.00 47.44 ATOM 2329 OD1 ASNA 354 19.467 31.036 -7.474 1.00 47.44 ATOM 2331 N GLN A 355 22.999 32.621 -4.419 1.00 37.62 ATOM 2332 C GLN A 355 24.371 33.042 -4.128 1.00 32.57 ATOM 2332 C GLN A 355 24.371 33.042 -4.128 1.00 32.57 ATOM 2333 C GLN A 355 22.999 32.621 -4.419 1.00 37.62 ATOM 2333 C GLN A 355 24.371 33.042 -4.128 1.00 32.57 ATOM 2334 C GLN A 355 24.371 33.042 -4.128 1.00 34.85 ATOM 2335 CB GLN A 355 24.371 33.042 -4.128 1.00 32.57 ATOM 2334 C GLN A 355 25.899 32.621 -4.419 1.00 37.62 ATOM 2335 CB GLN A 355 25.899 32.621 -4.419 1.00 37.62 ATOM 2336 CG GLN A 355 25.899 32.621 -4.419 1.00 39.05 ATOM 2337 CD GLN A 355 25.899 32.621 -4.419 1.00 39.05 ATOM 2337 CD GLN A 355 25.899 32.711 -2.597 1.00 29.33 ATOM 2334 C GLN A 355 25.899 32.711 -4.999 1.00 40.57 ATOM 2340 N SER A 356 26.419 31.514 -1.304 1.00 25.71 ATOM 2340 N SER A 356 26.419 31.514 -1.304 1.00 25.71 ATOM 2340 N SER A 356 26.419 31.514 -1.304 1.00 25.71 ATOM 2340 N SER A 356 26.419 31.514 -1.304 1.00 25.71 ATOM 2340 N SER A 356 26.419 31.514 -1.304 1.00 25.71 ATOM 2345 CG SER A 356 27.850 31.897 -0.981 1.00 24.59 ATOM 2347 CA PHE A 357 28.667 31.583 0.239 1.00 20.53 ATOM 2347 CA PHE A 357 29.679 31.			CB	VAL	A 352	22.	456 3	7.767	-2.939	1.00	38.31
ATOM 2315 CG2 VAL A 352										1.00	38.33
ATOM 2316 N THR A 353											
ATOM 2317 CA THR A 353											
ATOM 2318 C THR A 353											
ATOM 2319 O THR A 353											
ATOM 2320 CB THR A 353	MOTA	2318									
ATOM 2321 OG1 THR A 353	MOTA	2319	O	THR :	A 353	20.	941 3	4.536	-5.688		
ATOM 2322 CG2 THR A 353	ATOM	2320	CB	THR :	A 353	17.	929 3	4.672	-4.578	1.00	45.29
ATOM 2322 CG2 THR A 353	ATOM	2321	OG1	THR :	A 353	18.	018 3	5.743	-5.526	1.00	46.63
ATOM 2323 N ASN A 354 20.307 32.507 -4.839 1.00 42.20 ATOM 2324 CA ASN A 354 21.183 31.741 -5.742 1.00 43.39 ATOM 2325 C ASN A 354 22.641 32.166 -5.611 1.00 41.22 ATOM 2326 O ASN A 354 20.698 31.887 -7.187 1.00 45.64 ATOM 2327 CB ASN A 354 20.698 31.887 -7.187 1.00 45.64 ATOM 2329 OD1 ASN A 354 19.467 31.036 -7.474 1.00 47.44 ATOM 2329 OD1 ASN A 354 19.467 31.036 -7.474 1.00 47.44 ATOM 2329 OD1 ASN A 354 19.467 31.036 -6.534 1.00 47.73 ATOM 2331 N GLN A 355 22.999 32.621 -4.419 1.00 37.62 ATOM 2332 CA GLN A 355 24.371 33.042 -4.128 1.00 34.85 ATOM 2333 C GLN A 355 24.371 33.042 -4.128 1.00 34.85 ATOM 2333 C GLN A 355 24.737 32.475 -2.764 1.00 32.57 ATOM 2334 O GLN A 355 24.4737 32.475 -2.764 1.00 32.57 ATOM 2335 CB GLN A 355 24.459 34.563 -4.105 1.00 35.77 ATOM 2336 CG GLN A 355 25.834 35.089 -3.797 1.00 38.04 ATOM 2337 CD GLN A 355 25.834 35.089 -3.797 1.00 38.04 ATOM 2338 OEI GLN A 355 25.834 35.089 -3.797 1.00 39.05 ATOM 2338 OEI GLN A 355 25.586 37.171 -4.992 1.00 40.57 ATOM 2338 OEI GLN A 355 25.586 37.171 -4.992 1.00 39.05 ATOM 2338 OEI GLN A 355 25.586 37.171 -4.992 1.00 39.05 ATOM 2340 N SER A 356 25.989 32.071 -2.597 1.00 29.33 ATOM 2341 CA SER A 356 26.419 31.514 -1.304 1.00 25.60 ATOM 2342 C SER A 356 26.419 31.514 -1.304 1.00 25.60 ATOM 2343 O SER A 356 26.313 29.991 -1.318 1.00 25.71 ATOM 2340 N PHE A 357 28.267 31.583 0.239 1.00 20.53 ATOM 2344 CB SER A 356 26.313 29.991 -1.318 1.00 25.71 ATOM 2346 N PHE A 357 28.267 31.583 0.239 1.00 20.53 ATOM 2344 CB SER A 356 26.313 29.991 -1.318 1.00 25.71 ATOM 2346 N PHE A 357 28.267 31.583 0.239 1.00 20.53 ATOM 2347 CA PHE A 357 29.639 31.865 0.676 1.00 17.95 ATOM 2348 C PHE A 357 29.639 31.865 0.676 1.00 17.55 ATOM 2349 O PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2351 CG PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2351 CG PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2351 CG PHE A 357 29.687 33.126 1.550 1.00 17.61								4.988	-3.551	1.00	46.31
ATOM 2324 CA ASN A 354 21.183 31.741 -5.742 1.00 43.39 ATOM 2325 C ASN A 354 22.641 32.166 -5.611 1.00 41.22 ATOM 2326 O ASN A 354 22.641 32.166 -5.611 1.00 41.22 ATOM 2327 CB ASN A 354 20.698 31.887 -7.187 1.00 45.64 ATOM 2329 OD1 ASN A 354 19.467 31.036 -7.474 1.00 47.44 ATOM 2329 OD1 ASN A 354 19.467 31.036 -7.474 1.00 47.44 ATOM 2329 OD1 ASN A 354 19.121 30.159 -6.534 1.00 47.73 ATOM 2331 N GLN A 355 22.999 32.621 -4.419 1.00 37.62 ATOM 2332 CA GLN A 355 24.371 33.042 -4.128 1.00 34.85 ATOM 2333 C GLN A 355 24.737 32.475 -2.764 1.00 32.57 ATOM 2334 O GLN A 355 24.4737 32.475 -2.764 1.00 32.57 ATOM 2335 CB GLN A 355 24.459 34.563 -4.105 1.00 35.77 ATOM 2337 CD GLN A 355 25.834 35.089 -3.797 1.00 38.04 ATOM 2337 CD GLN A 355 25.834 35.089 -3.797 1.00 38.04 ATOM 2338 OEI GLN A 355 25.909 36.590 -3.915 1.00 39.05 ATOM 2339 NE2 GLN A 355 25.586 37.171 -4.992 1.00 40.57 ATOM 2339 NE2 GLN A 355 25.989 32.071 -2.597 1.00 29.33 ATOM 2341 CA SER A 356 26.419 31.514 -1.304 1.00 25.60 ATOM 2342 C SER A 356 26.419 31.514 -1.304 1.00 25.71 ATOM 2343 O SER A 356 26.313 29.991 -1.318 1.00 22.66 ATOM 2344 CB SER A 356 26.313 29.991 -1.318 1.00 22.66 ATOM 2344 CB SER A 356 26.313 29.991 -1.318 1.00 25.71 ATOM 2347 CA PHE A 357 29.687 31.583 0.239 1.00 20.53 ATOM 2348 C PHE A 357 29.687 33.126 1.550 1.00 17.95 ATOM 2349 O PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2349 O PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2349 O PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2345 CB PHE A 357 29.687 33.126 1.550 1.00 17.62											
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ATOM 2347 CA PHE A 357 29.639 31.865 0.676 1.00 17.95 ATOM 2348 C PHE A 357 30.104 30.643 1.437 1.00 17.15 ATOM 2349 O PHE A 357 29.279 29.750 1.784 1.00 17.21 ATOM 2350 CB PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2351 CG PHE A 357 28.926 33.017 2.850 1.00 17.61	MOTA										
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ATOM 2348 C PHE A 357 30.104 30.643 1.437 1.00 17.15 ATOM 2349 O PHE A 357 29.279 29.750 1.784 1.00 17.21 ATOM 2350 CB PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2351 CG PHE A 357 28.926 33.017 2.850 1.00 17.61			CA	PHE .	A 357	29.	639 3	1.865	0.676		
ATOM 2349 O PHE A 357 29.279 29.750 1.784 1.00 17.21 ATOM 2350 CB PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2351 CG PHE A 357 28.926 33.017 2.850 1.00 17.61								0.643	1.437	1.00	17.15
ATOM 2350 CB PHE A 357 29.687 33.126 1.550 1.00 17.62 ATOM 2351 CG PHE A 357 28.926 33.017 2.850 1.00 17.61											
ATOM 2351 CG PHE A 357 28.926 33.017 2.850 1.00 17.61											
ATOM 2552 CDI PRE A 557 29.571 52.625 4.010 15.09											
	ATOM	2332	CDI	rns .	וכנ מ	29.	J / L 3	2.023	3.010	1.00	,,

ATOM	2353	CD2	PHE A	357	27.57	7 33.357	2.912	1.00 16.90
ATOM	2354		PHE A		28.88			1.00 14.87
		-						
MOTA	2355	CE2	PHE A		26.88		4.120	1.00 15.64
ATOM	2356	CZ	PHE A	357	27.53	8 32.924	5.280	1.00 16.14
ATOM	2357	N	ARG A		31.39	7 30.545	1.687	1.00 16.29
ATOM	2358	CA	ARG A		31.89		2.412	1.00 14.04
MOTA	2359	С	ARG A	358	32.64	2 29.755	3.664	1.00 14.59
ATOM	2360	0	ARG A	358	33.23	7 30.869	3.785	1.00 13.01
MOTA	2361	CB	ARG A		32.78			1.00 14.11
MOTA	2362	CG	ARG A	358	34.08	4 29.172	1.102	1.00 13.28
ATOM	2363	CD	ARG A	358	34.80	9 28.275	0.121	1.00 13.06
			ARG A		36.09		-0.291	1.00 14.39
MOTA	2364	NE						
ATOM	2365	cz	ARG A	. 358	36.72	3 28.489	-1.409	1.00 14.92
ATOM	2366	NH1	ARG A	358	36.18	8 27.591	-2.232	1.00 13.71
ATOM	2367	NH2			37.88	8 29.045	-1.701	1.00 12.88
							4.596	
MOTA	2368	N	ILE A		32.61			1.00 14.51
ATOM	2369	CA	ILE A	. 359	33.26	8 28.935	5.891	1.00 16.36
ATOM	2370	С	ILE A	359	34.24	2 27.762	5.913	1.00 15.41
ATOM	2371	ō	ILE A		33.83		5.675	1.00 15.49
ATOM	2372	CB	ILE A		32.19		7.001	1.00 17.94
MOTA	2373	CG1	ILE A	. 359	31.54	30.190	7.198	1.00 19.68
ATOM	2374	CG2	ILE A	359	32.76	6 28.260	8.255	1.00 20.12
					32.51		7.500	1.00 22.40
MOTA	2375	CD1	ILE A					
MOTA	2376	N	THR A	. 360	35.51	3 28.046	6.162	1.00 13.01
ATOM	2377	CA	THR A	360	36.53	1 26.983	6.167	1.00 14.32
ATOM	2378	C	THR A		37.30	7. 26.894	7.470	1.00 14.04
MOTA	2379		THR A		37.89		7.938	1.00 13.82
MOTA	2380	CB	THR A	360	37.53	5 27.202	5.021	1.00 14.49
ATOM	2381	OG1	THR A	360	36.82	3 27.286	3.774	1.00 15.69
		CG2			38.53		4.964	1.00 15.11
ATOM	23,82		THR A					
MOTA	2383	N	ILE A	361	37.33	25.709	8.074	1.00 13.79
ATOM	2384	ÇA	ILE A	361	38.09	25.524	9.330	1.00 17.36
ATOM	2385	C	ILE A		. 39.24		9.122	1.00 16.53
MOTA	2386	0	ILE A		39.23		8.160	1.00 16.37
MOTA	2387	CB	ILE A	361	37.20	3 24.982	10.476	1.00 18.15
ATOM	2388	CG1	ILE A	361	36.60	3 23.632	10.077	1.00 18.53
ATOM	2389	CG2	ILE A		36.12		10.830	1.00 18.95
ATOM	2390	CD1	ILE A		35.899		11.208	1.00 18.19
MOTA	2391	N	LEU A	362	40.23	24.614	9.998	1.00 17.82
ATOM	2392	CA	LEU A	362	41.37	23.710	9.876	1.00 18.92
ATOM	2393	C	LEU A		41.412		10.983	1.00 17.87
MOTA	2394	0	LEU A		40.533	22.654	11.912	1.00 17.21
MOTA	2395	CB	LEU A	362	42.679	24.525	9.837	1.00 22.47
ATOM	2396	CG	LEU A		42.686		10.320	1.00 25.03
			LEU A		42.949		11.802	1.00 28.14
ATOM	2397							
MOTA	2398	CD2	LEU A		43.783		9.623	1.00 25.06
MOTA	2399	N	PRO A	363	42.380	21.729	10.910	1.00 16.12
ATOM	2400	CA	PRO A		42.50		11.925	1.00 14.51
			PRO A				13.303	1.00 14.50
ATOM	2401	С			42.628			
MOTA	2402	0	PRO A		42.23		14.339	1.00 13.48
ATOM	2403	CB	PRO A	363	43.803	19.971	11.534	1.00 15.57
ATOM	2404	CG	PRO A		43.902		10.076	1.00 16.87
								1.00 14.60
MOTA	2405	CD	PRO A		43.450		9.903	
ATOM	2406	N	GLN A		43.178		13.337	1.00 12.36
ATOM	2407	CA	GLN A	364	43.357	23.271	14.608	1.00 13.04
			GLN A		42.014		15.254	1.00 13.41
MOTA	2408	C						
MOTA	2409	0	GLN A		41.953		16.467	1.00 12.73
ATOM	2410	CB	GLN A	364	44.11	L 24.585	14.392	1.00 12.04
ATOM	2411	CG	GLN A		45.637		14.304	1.00 11.85
		CD	GLN A		46.141		12.919	1.00 11.11
MOTA	2412							
ATOM	2413		GLN A		47.372		12.625	1.00 13.65
ATOM	2414	NE2	GLN A	364	45.245	23.621	12.056	1.00 8.04
							*	

MOTA	2415	N	GLN	Α	365	40.939	23.446	14.478	1.00 13.30
MOTA	2416	CA	GLN	А	365	39.580	23.657	15.023	1.00 14.36
MOTA	2417	C	GLN			38.873	22.341	15.339	1.00 14.57
	2418		GLN			38.312	22.175	16.457	1.00 16.56
MOTA		0							
MOTA	2419	CB	GLN			38.691	24.452	14.056	1.00 14.03
MOTA	2420	CG	GLN			38.816	25.962	14.167	
MOTA	2421	CD	GLN	А	365	40.073	26.489	13.515	1.00 15.81
MOTA	2422	OE1	GLN	Α	365	40.290	26.292	12.282	1.00 15.51
MOTA	2423	NE2	GLN	Α	365	40.917	27.158	14.295	1.00 15.82
ATOM	2424	N	TYR			38.873	21.392	14.406	1.00 14.93
ATOM	2425	CA	TYR			38.149	20.128	14.673	1.00 15.12
						38.914		15.447	1.00 15.66
ATOM	2426	C	TYR					15.703	
MOTA	2427	0	TYR			38.378	17.930		1.00 17.42
MOTA	2428	CB	TYR			37.557	19.567	13.371	1.00 14.28
MOTA	2429	CG	TYR			38.541	19.107	12.322	1.00 13.05
MOTA	2430	CD1	TYR	Α	366	39.228	17.907	12.467	1.00 13.67
MOTA	2431	CD2	TYR	Α	366	38.721	19.835	11.145	1.00 13.44
ATOM	2432	CE1	TYR	A	366	40.062	17.431	11.463	1.00 12.91
MOTA	2433	CE2	TYR			39.555	19.369	10.128	1.00 12.63
ATOM	2434	CZ	TYR			40.218	18.163	10.294	1.00 13.86
MOTA	2435	OH	TYR			41.008	17.669	9.287	1.00 12.42
ATOM	2436	N	LEU			40.144	19.367	15.835	1.00 16.84
						40.966	18.450	16.660	1.00 16.98
ATOM	2437	CA	LEU						1.00 17.50
ATOM	2438	C	LEU			40.996	19.161	18.017	
MOTA	2439	0	LEU			41.662	20.224	18.172	1.00 16.40
MOTA	2440	CB	LEU			42.382	18.324	16.088	1.00 17.44
ATOM	2441	CG	LEU			42.764	16.991	15.429	1.00 18.54
MOTA	2442	CD1	LEU	Α	367	41.681	16.534	14.482	1.00 17.60
MOTA	2443	CD2	LEU	A	367	44.091	17.143	14.700	1.00 17.38
MOTA	2444	N	ARG			40.270	18.624	18.990	1.00 17.06
MOTA	2445	CA	ARG			40.192	19.253	20.326	1.00 17.22
MOTA	2446	C	ARG			41.341	18.874	21.243	1.00 16.52
	2447	Ö	ARG			41.554	17.662	21.538	1.00 16.19
MOTA							18.871	21.009	1.00 16.02
MOTA	2448	CB	ARG			38.879			1.00 10.02
ATOM	2449	CG	ARG			38.050	20.055	21.444	
ATOM	2450	CD	ARG			37.415	19.811	22.792	1.00 17.88
MOTA	2451	NE	ARG			36.840	18.474	22.906	1.00 17.20
ATOM	2452	CZ	ARG			36.775	17.806	24.053	1.00 18.65
ATOM	2453		ARG			37.247	18.361	25.164	1.00 18.77
MOTA	2454	NH2	ARG	A	368	36.258	16.584	24.095	1.00 17.53
ATOM	2455	N	PRO	Α	369	42.100	19.867	21.722	1.00 17.88
MOTA	2456	CA	PRO			43.220	19.558	22.615	1.00 19.69
MOTA	2457	С	PRO	А	369	42.744		23.969	1.00 22.16
MOTA	2458	ō	PRO			41.786	19.645	24.575	1.00 20.49
MOTA	2459	СВ	PRO			43.983	20.883	22.700	1.00 20.03
	2460	CG	PRO			42.932	21.911	22.429	1.00 19.96
ATOM	_	CD	PRO			42.122	21.285	21.320	1.00 17.42
MOTA	2461							24.444	1.00 23.75
MOTA	2462	N	VAL			43.376	18.001		1.00 27.84
MOTA	2463	CA	VAL			43.040	17.399	25.747	
MOTA	2464	С	VAL			44.332	16.921	26.394	1.00 30.26
ATOM	2465	0	VAL	A	370	45.321	16.577	25.682	1.00 30.79
ATOM	2466	CB	VAL	А	370	42.093	16.197	25.577	1.00 26.52
MOTA	2467	CG1	VAL	Α	370	40.771	16.654	24.989	1.00 26.57
ATOM	2468		VAL			42.737	15.160	24.669	1.00 26.53
MOTA	2469	N	GLU			44.361	16.891	27.719	1.00 35.50
ATOM	2470	CA	GLU			45.574	16.450	28.426	1.00 40.60
ATOM	2471	C	GLU			45.800	14.963	28.235	1.00 42.42
	2472	0	GLU			44.832	14.138	28.321	1.00 41.89
MOTA			GLU			45.472	16.758	29.921	1.00 43.12
ATOM	2473	CB						30.443	1.00 47.33
MOTA	2474	CG	GLU			46.603	17.634	29.864	1.00 49.98
MOTA	2475	CD	GLU			47.954	17.245	29.804	1.00 49.98
MOTA	2476	OE1	GLU	A	3 / I	48.264	16.036	23.010	T.00 JI.03

ATOM	2477	OE2	GLU	Α	371	48.710	18.151	29.456	1.00 51.00
ATOM	2478	N	ASP	Α	372	47.046	14.596	27.960	1.00 45.77
ATOM	2479	CA	ASP			47.396	13.182	27.774	1.00 49.75
ATOM	2480	C	ASP			46.889	12.468	29.014	1.00 52.41
	2481					47.090	12.966	30.165	1.00 52.32
ATOM		0	ASP						
ATOM	2482	CB	ASP			48.913	13.015	27.665	1.00 50.28
MOTA	2483	CG	ASP			49.323	11.587	27.333	1.00 51.15
MOTA	2484	OD1	ASP	Α	372	50.541	11.323	27.246	1.00 51.32
MOTA	2485	OD2	ASP	Α	372	48.429	10.729	27.156	1.00 50.76
ATOM	2486	N	VAL	Α	373	46.217	11.340	28.819	1.00 55.35
ATOM	2487	CA	VAL	Α	373	45.688	10.570	29.956	1.00 58.73
ATOM	2488	C	VAL			46.850	10.213	30.896	1.00 60.04
MOTA.	2489		VAL			47.465	9.105	30.817	1.00 60.06
ATOM	2490	CB	VAL			44.901	9.313	29.433	1.00 59.43
						45.292	8.044	30.176	1.00 59.64
ATOM	2491	CG1	VAL						1.00 59.89
ATOM	2492	CG2	VAL			43.402	9.556	29.597	
ATOM	2493	N	ALA			47.187	11.169	31.759	1.00 61.58
ATOM	2494	CA	ALA			48.277	11.020	32.755	1.00 61.52
MOTA	2495	С	ALA			49.709	11.205	32.233	1.00 61.38
MOTA	2496	0	ALA	A	374	50.104	10.633	31.169	1.00 60.95
MOTA	2497	CB	ALA	Α	374	48.155	9.668	33.455	1.00 62.66
ATOM	2498	N	THR	Α	375	50.477	12.002	32.977	1.00 61.03
ATOM	2499	CA	THR	A	375	51.919	12.320	32.715	1.00 60.30
ATOM	2500	С	THR	Α	375	52.401	12.358	31.269	1.00 58.41
ATOM	2501	0	THR	Α	375	52.361	11.308	30.555	1.00 59.21
ATOM	2502	СB	THR			52.838	11.327	33.455	1.00 61.35
MOTA	2503	OG1	THR			52.302	11.049	34.756	1.00 62.26
ATOM	2504	CG2	THR			54.237	11.912	33.599	1.00 61.47
MOTA	2505	N	SER			52.892	13.520	30.833	1.00 55.18
ATOM	2506	CA	SER			53.407	13.683	29.445	1.00 51.40
MOTA	2507	C	SER			53.538	15.132	28.981	1.00 48.79
			SER			52.887	16.067	29.540	1.00 48.19
ATOM	2508	0				52.502	12.943	28.456	1.00 51.90
MOTA	2509	CB	SER					27.115	1.00 51.94
ATOM	2510	OG:	SER			52.880	13.193		1.00 44.88
ATOM	2511	N	GLN			54.373	15.333	27.968	1.00 41.28
MOTA	2512	CA	GLN			54.576	16.664	27.367	
ATOM	2513	С	GLN			54.106	16.580	25.923	1.00 37.22
MOTA	2514	0	GLN			54.380	17.489	25.081	1.00 35.23
MOTA	2515	CB	GLN			56.048	17.062	27.425	1.00 43.59
MOTA	2516	CG	GLN			56.468	17.585	28.789	1.00 46.22
MOTA	2517	CD	GLN	A	377	57.955	17.831	28.886	1.00 47.12
MOTA	2518		. GLN			58.710	17.710	27.867	1.00 48.44
MOTA	2519	NE2	GLN	A	377	58.414	18.177	30.081	1.00 48.23
MOTA	2520	N	ASP	A	378	53.399	15.499	25.618	1.00 31.89
MOTA	2521	CA	ASP	Α	378	52.866	15.289	24.263	1.00 28.31
MOTA	2522	C	ASP	A	378	51.663	16.183	24.034	1.00 25.36
MOTA	2523	0	ASP	Α	378	50.958	16.590	25.004	1.00 22.58
MOTA	2524	CB	ASP	Α	378	52.422	13.835	24.072	1.00 28.64
MOTA	2525	CG	ASP			53.582	12.867	23.998	1.00 29.19
MOTA	2526		ASP			54.746	13.316	23.948	1.00 30.91
ATOM	2527		ASP			53.323	11.647	23.981	1.00 30.50
ATOM	2528	N	ASP			51.415	16.513	22.776	1.00 23.06
ATOM	2529	CA	ASP			50.236	17.317	22.436	1.00 22.51
ATOM	2530	C	ASP			49.220	16.294	21.964	1.00 21.46
MOTA	2531		ASP			49.436	15.581	20.945	1.00 19.87
						50.570	18.335	21.346	1.00 21.72
ATOM	2532	CB	ASP				19.377	21.829	1.00 23.29
MOTA	2533	CG	ASP			51.557	19.786	23.005	1.00 23.29
MOTA	2534		ASP			51.434		23.003	1.00 23.50
MOTA	2535		ASP			52.446	19.789		1.00 20.99
MOTA	2536	И	CYS			48.128	16.182	22.706	1.00 20.99
ATOM	2537	CA	CYS			47.082	15.201	22.393	1.00 20.40
MOTA	2538	С	CYS	A	380	45.769	15.865	22.013	1.00 17.74

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ATOM	2539	0	CYS A	380	45.489	17.038	22.417	1.00 18.77
ATOM	2540	CB	CYS A	380	46.867	14.292	23.596	1.00 23.14
ATOM	2541	SG	CYS A		48.368	13.550	24.327	1.00 25.25
	•						21.255	1.00 18.49
MOTA	2542	N	TYR A		44.947	15.140		
MOTA	2543	CA	TYR A		43.656	15.681	20.785	1.00 17.31
MOTA	2544	C	TYR A	381	42.595	14.610	20.602	1.00 17.45
MOTA	2545	0	TYR A	381	42.890	13.376	20.532	1.00 16.46
ATOM	2546	СВ	TYR A		43.833	16.370	19.427	1.00 15.47
ATOM	2547	CG	TYR A		45.034	17.275	19.314	1.00 14.93
					44.899	18.659	19.408	1.00 14.20
MOTA	2548	CD1	TYR A					
ATOM	2549	CD2	TYR A		46.311	16.746	19.118	1.00 14.17
MOTA	2550	CE1	TYR A		46.009	19.499	19.307	1.00 14.66
MOTA	2551	CE2	TYR A	381	47.431	17.576	19.021	1.00 15.73
ATOM	2552	CZ	TYR A	381	47.272	18.952	19.113	1.00 16.02
MOTA	2553	OH	TYR A	381	48.369	19.785	18.994	1.00 15.32
ATOM	2554	N	LYS A	382	41.356	15.066	20.506	1.00 18.35
ATOM	2555	CA	LYS A		40.218	14.174	20.248	1.00 20.26
		C	LYS A		39.555	14.695	18.981	1.00 19.31
MOTA	2556							
MOTA	2557	0	LYS A		39.575	15.941	18.704	1.00 19.65
MOTA	2558	CB	LYS A		39.221	14.204	21.404	1.00 21.74
MOTA	2559	CG	LYS A		39.632	13.348	22.585	1.00 25.42
MOTA	2560	CD	LYS A	382	38.509	13.266	23.602	1.00 27.59
ATOM	2561	CE	LYS A	382	38.878	12.342	24.759	1.00 29.84
ATOM	2562	NZ	LYS A	382	37.779	12.246	25.761	1.00 31.22
ATOM	2563	N	PHE A		38.994	13.786	18.192	1.00 18.55
MOTA	2564	CA	PHE A		38.298	14.165	16.942	1.00 16.97
					36.992	14.823	17.375	1.00 16.22
MOTA	2565	C	PHE A					
ATOM	2566	0	PHE A		36.079	14.138	17.908	1.00 13.73
MOTA	2567	CB	PHE A		38.026	12.907	16.110	1.00 16.57
ATOM	2568	CG	PHE A	383	37.447	13.182	14.750	1.00 16.49
MOTA	2569	CD1	PHE A	383	38.052	14.091	13.890	1.00 14.48
MOTA	2570	CD2	PHE A	383	36.319	12.489	14.308	1.00 15.06
ATOM	2571	CE1	PHE A		37.542	14.306	12.606	1.00 16.02
ATOM	2572	CE2	PHE A		35.807	12.696	13.029	1.00 15.64
		CZ	PHE A		36.419	13.603	12.176	1.00 15.10
MOTA	2573				36.885	16.134	17.173	1.00 16.28
MOTA	2574	N	ALA A					
ATOM	2575	CA	ALA A		35.675	16.893	17.586	1.00 15.54
MOTA	2576	C	ALA A		34.549,	16.931	16.559	1.00 15.46
MOTA	2577	0	ALA A		33.768	17.931	16.487	1.00 15.60
MOTA	2578	CB	ALA A	384	36.061	18.316	17.987	1.00 14.96
ATOM	2579	N	ILE A	385	34.451	15.888	15.745	1.00 14.66
ATOM	2580	CA	ILE A	385	33.356	15.792	14.763	1.00 13.45
MOTA	2581	C	ILE A		32.651	14.487	15.093	1.00 14.39
ATOM	2582	ŏ	ILE A		33.303	13.410	15.179	1.00 12.37
ATOM	2583	СВ	ILE A		33.862	15.724	13.315	1.00 12.54
					34.696	16.959	12.988	1.00 13.08
ATOM	2584	CG1	-					1.00 12.56
ATOM	2585	CG2	ILE A		32.675	15.655	12.367	
MOTA	2586	CD1	ILE A		35.178	17.003	11.549	1.00 10.74
MOTA	2587	N	SER A		31.343	14.543	15.297	1.00 14.95
MOTA	2588	CA	SER A	386	30.605	13.319	15.637	1.00 16.99
MOTA	2589	С	SER A	386	29.275	13.221	14.918	1.00 17.48
ATOM	2590	0	SER A		28.795	14.207	14.279	1.00 18.09
ATOM	2591	СВ	SER A		30.385	13.240	17.151	1.00 16.69
ATOM	2592	OG	SER A		29.630	14.345	17.616	1.00 16.81
							15.016	1.00 19.86
MOTA	2593	N	GLN A		28.673	12.044		
MOTA	2594	CA	GLN A		27.384	11.748		1.00 23.09
MOTA	2595	С	GLN A		26.209	12.317	15.160	1.00 22.61
MOTA	2596	0	GLN A	387	26.221	12.363	16.427	1.00 22.90
ATOM	2597	CB	GLN A	387	27.222	10.234		1.00 24.53
MOTA	2598	CG	GLN A	387	26.035	9.795	13.411	1.00 28.94
ATOM	2599	CD	GLN A	387	25.971	8.286	13.272	1.00 30.39
ATOM	2600		GLN A		27.013	7.619	12.999	1.00 31.54
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MOTA	2601	NE2	GLN	Α	387	24.782	7.721	13.441	1.00	32.07
ATOM	2602	N	SER			25.186	12.743	14.434	1.00	21.60
MOTA	2603	CA	SER			23.981	13.306	15.055	1.00	21.59
MOTA	2604	С	SER	Α	388	22.728	12.711	14.429	1.00	22.68
MOTA	2605	0	SER			22.707	12.380	13.203		23.08
ATOM	2606	СВ	SER	Α	388'	23.959	14.824	14.871	1.00	19.88
ATOM	2607	OG.	SER			22.661	15.342	15.112		19.18
ATOM	2608	N	SER			21.681	12.551	15.227		23.51
ATOM	2609	CA	SER			20.405	12.024	14.690	1.00	24.44
ATOM	2610	С	SER	A	389	19.391	13.167	14.708	1.00	23.83
ATOM	2611	0	SER	Α	389	18.181	12.973	14.385	1.00	23.81
ATOM	2612	CB	SER			19.902	10.847	15.534	1.00	25.63
MOTA	2613	OG	SER	Α	389	19.681	11.235	16.881	1.00	27.65
MOTA	2614	N	THR	A	390	19.861	14.360	15.066	1.00	22.66
MOTA	2615	CA	THR	A	390	18.984	15.553	15.127	1.00	22.60
ATOM	2616	С	THR	Α	390	19.471	16.709	14.260	1.00	21.12
ATOM	2617	0	THR	Α	390	19.272	17.910	14.608	1.00	21.35
MOTA	2618	CB	THR	Α	390	18.825	16.052	16.577	1.00	23.02
ATOM	2619	OG1	THR	Α	390	20.117	16.288	17.150	1.00	24.55
MOTA	2620	CG2	THR	A	390	18.079	15.010	17.413	1.00	23.83
MOTA	2621	N	GLY			20.093	16.381	13.136		19.75
ATOM	2622	CA	GLY			20.573	17.410	12.237		16.88
MOTA	2623	C	GLY	A	391	21.982	17.891	12.526		17.24
ATOM	2624	0	GLY			22.672		13.472		16.27
MOTA	2625	N	THR			22.427	18.851	11.730		14.99
ATOM	2626	CA	THR			23.773	19.423	11.880		14.81
ATOM	2627	C	THR			23.841	20.514	12.938		14.47
MOTA	2628	0	THR			22.949	21.409	13.012		16.11
MOTA	2629	CB	THR			24.266	20.062	10.564		12.95
ATOM	2630	OG1				24.494	19.043	9.588		14.51
MOTA	2631	CG2	THR			25.572	20.839	10.800		14.09
ATOM	2632	N	VAL			24.857	20.458	13.779		13.06
ATOM	2633	CA	VAL			25.027	21.534	14.746		15.07
ATOM	2634	C	VAL			26.462	22.033	14.684		15.47
ATOM	2635	0	VAL			27.450	21.265	14.908		16.85
MOTA	2636	CB	VAL			24.619	21.128	16,201		16.35
ATOM	2637		VAL			24.559	19.624	16.348		15.06 13.79
MOTA	2638		VAL MET			25.566 26.592	21.766	17.210 14.312		15.41
ATOM	2639 2640	N	MET			27.900	23.298	14.231		16.55
ATOM ATOM	2641	CA C	MET			28.188	24.442	15.647		16.43
ATOM	2642	0	MET			27.737	25.553	16.059		14.99
ATOM	2643	CB	MET			27.822	25.143	13.264	1.00	
ATOM	2644	CG	MET			27.607	24.724	11.818	1.00	
	2645	SD	MET			27.178	26.083	10.700	1.00	
ATOM	2646	CE	MET			25.475	25.768	10.522	1.00	
ATOM	2647	N	GLY			28.909	23.622	16.406	1.00	
ATOM	2648	CA	GLY			29.220	23.967	17.780	1.00	
ATOM	2649	С	GLY			30.487	24.775	17.971	1.00	
MOTA	2650	0	GLY			31.011	25.408	17.005	1.00	16.25
ATOM	2651	N	ALA			30.989	24.769	19.202	1.00	17.29
ATOM	2652	CA	ALA			32.211	25.511	19.586	1.00	19.21
MOTA	2653	C	ALA			33.383	25.310	18.634	1.00	19.63
MOTA	2654	0	ALA			34.050	26.303	18.223	1.00	22.56
ATOM	2655	CB	ALA			32.626	25.128	21.013	1.00	16.95
MOTA	2656	N	VAL			33.661	24.065	18.269	1.00	21.31
ATOM	2657	CA	VAL	A	397	34.792	23.781	17.353	1.00	
MOTA	2658	С	VAL	Α	397	34.690	24.592	16.068	1.00	
ATOM	2659	0	VAL			35.731	25.029	15.496	1.00	
MOTA	2660	CB	VAL			34.874	22.274	17.012	1.00	
MOTA	2661		VAL			35.065	21.480	18.287	1.00	
MOTA	2662	CG2	VAL	A	397	33.623	21.826	16.290	1.00	25.89

MOTA	2663	N	ILE A	398	33.472	24.805	15.586	1.00 21.78
MOTA	2664	CA	ILE A	398	33.276	25.612	14.359	1.00 21.50
ATOM	2665	C	ILE A		33.403	27.086	14.735	1.00 19.91
ATOM	2666	ō	ILE A		34.222	27.849	14.135	1.00 16.77
MOTA	2667	CB	ILE A		31.872	25.390	13.749	1.00 23.48
MOTA	2668	CG1	ILE A		31.859	24.113	12.910	1.00 26.70
ATOM .	2669	CG2	ILE A	398	31.469	26.596	12.895	1.00 24.67
ATOM	2670	CD1	ILE A	398	32.656	24.223	11.620	1.00 27.64
ATOM	2671	N	MET A		32.614	27.492	15.726	1.00 17.64
ATOM	2672	CA	MET A		32.594	28.889	16.201	1.00 16.99
					33.951	29.439	16.640	1.00 17.65
ATOM	2673	C	MET A					
MOTA	2674	0	MET A		34.202	30.677	16.517	1.00 18.70
MOTA	2675	CB	MET A		31.575	29.025	17.331	1.00 15.33
ATOM	2676	CG	MET A	399	30.138	28.800	16.866	1.00 14.30
ATOM	2677	SD	MET A	399 -	28.891	29.038	18.155	1.00 16.41
MOTA	2678	CE	MET A	399	28.972	30.826	18.388	1.00 10.15
ATOM	2679	N	GLU A		34.835	28.579	17.143	1.00 16.09
ATOM	2680	CA	GLU A		36.175	29.051	17.580	1.00 16.46
	2681	C	GLU A		36.968	29.576	16.389	1.00 14.50
ATOM								1.00 14.83
MOTA	2682	0	GLU A		37.971	30.332	16.553	
MOTA	2683	CB	GLU A		36.957	27.919	18.257	1.00 15.95
ATOM	2684	CG	GLU A		36.318	27.419	19.540	1.00 18.44
ATOM	2685	CD	GLU A	400	37.156	26.376	20.243	1.00 18.72
ATOM	2686	OE1	GLU A	400	37.771	25.542	19.546	1.00 20.29
ATOM	2687	OE2	GLU A		37.186	26.383	21.493	1.00 19.60
ATOM	2688	N	GLY A		36.544	29.204	15.190	1.00 13.62
ATOM	2689	CA	GLY A		37.246	29.662	14.010	1.00 15.09
					36.747	31.010	13.533	1.00 16.28
ATOM	2690	С	GLY A					
ATOM	2691	0	GLY A		37.435	31.693	12.716	1.00 16.14
MOTA	2692	N	PHE A		35.591	31.438	14.033	1.00 14.90
MOTA	2693	CA	PHE A	402	35.018	32.712	13.572	1.00 15.01
ATOM	2694	С	PHE A	402	34.378	33.605	14.615	1.00 15.52
ATOM	2695	0	PHE A	402	34.078	33.185	15.777	1.00 16.47
MOTA	2696	CB	PHE A		33.966	32.424	12.495	1.00 14.48
ATOM	2697	CG	PHE A		34.381	31.364	11.522	1.00 15.64
		CD1	PHE A		34.126	30.021	11.785	1.00 14.91
ATOM	2698	CD2	PHE A			31.700	10.376	1.00 15.20
MOTA	2699	_			35.095			
MOTA	2700	CE1	PHE A		34.581	29.027	10.920	1.00 15.18
MOTA	2701	CE2	PHE A		35.555	30.717	9.507	1.00 15.72
ATOM	2702	CZ	PHE A	402	35.298	29.376	9.782	1.00 15.12
MOTA	2703	N	TYR A	403	34.168	34.847	14.208	1.00 15.73
MOTA	2704	CA	TYR A	403 -	33.474	35.837	15.039	1.00 15.81
ATOM	2705	С	TYR A	403	32.071	35.641	14.489	1.00 14.48
ATOM	2706	0	TYR A		31.846	35.789	13.250	1.00 15.47
ATOM	2707	СВ	TYR A		33.977	37.251	14.731	1.00 14.45
	2708	CG	TYR A		33.265	38.340	15.499	1.00 15.22
ATOM						38.152	16.834	1.00 14.85
MOTA	2709		TYR A		32.899			
ATOM	2710		TYR A		33.018	39.584	14.916	1.00 14.28
MOTA	2711	CE1	TYR A	403	32.311	39.175	17.569	1.00 15.25
MOTA	2712	CE2	TYR A	403		40.617	15.644	1.00 14.12
ATOM	2713	CZ	TYR A	403	32.086	40.406	16.967	1.00 15.72
MOTA	2714	OH	TYR A	403	31.525	41.427	17.697	1.00 18.09
MOTA	2715	N	VAL A		31.125	35.286	15.345	1.00 14.70 .
MOTA	2716	CA	VAL A		29.753	35.040	14.854	1.00 14.44
		C			28.759	36.079	15.342	1.00 14.92
MOTA	2717		VAL A					
MOTA	2718	0	VAL A		28.552	36.259	16.582	1.00 15.62
MOTA	2719	CB	VAL A		29.284	33.629	15.260	1.00 14.39
MOTA	2720		VAL A		27.925	33.323	14.640	1.00 11.90
MOTA	2721	CG2	VAL A	404	30.327	32.603	14.819	1.00 12.73
MOTA	2722	N	VAL A	405	28.136	36.762	14.386	1.00 16.06
ATOM	2723	CA	VAL A	405	27.153	37.822	14.676	1.00 14.31
MOTA	2724	С	VAL A		25.717	37.312	14.562	1.00 16.79
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ATOM	2725	0	VAL A	405	25.238	36.955	13.443	1.00 16.14
MOTA	2726	CB	VAL A		27.318	39.004	13.700	1.00 13.66
		-	VAL A		26.302	40.092	14.021	1.00 12.39
ATOM	2727.							
MOTA	2728		VAL A		28.739	39.547	13.775	1.00 10.80
ATOM	2729	N	PHE A	406	25.019	37.260	15.691	1.00 16.73
ATOM	2730	CA	PHE A	406	23.616	36.805	15.685	1.00 16.71
ATOM	2731	C	PHE A		22.755	38.049	15.531	1.00 17.47
			PHE A		22.286	38.654	16.539	1.00 17.39
MOTA	2732	0						
MOTA	2733	CB	PHE A	406	23.287	36.053	16.979	1.00 13.96
MOTA	2734	CG	PHE A	406	24.061	34.765	17.139	1.00 13.82
MOTA	2735	CD1	PHE A	406	25.398	34.783	17.533	1.00 13.31
MOTA	2736	-	PHE A		23.464	33.538	16.863	1.00 12.85
	2737		PHE A		26.128	33.601	17.646	1.00 13.23
MOTA							16.973	1.00 12.78
ATOM	2738		PHE A		24.185	32.350		
MOTA	2739	CZ	PHE A		25.522	32.382	17.367	1.00 12.96
ATOM	2740	N	ASP A	407	22.566	38.449	14.278	1.00 18.08
ATOM	2741	CA	ASP A	407	21.785	39.647	13.932	1.00 19.70
ATOM	2742	C	ASP A		20.297	39.316	13.927	1.00 19.73
ATOM	2743	ō	ASP A		19.675	39.120	12.837	1.00 18.96
			ASP A		22.221	40.153	12.552	1.00 22.61
ATOM	2744	CB						
MOTA	2745	CG	ASP A		21.663	41.530	12.223	1.00 24.28
ATOM	2746	OD1	ASP A	407	20.660	41.935	12.849	1.00 24.12
MOTA	2747	OD2.	ASP A	407	22.225	42.198	11.325	1.00 23.37
ATOM	2748	N	ARG A	408	19.709	39.245	15.116	1.00 19.72
ATOM	2749	CA	ARG A		18.269	38.928	15.259	1.00 22.01
	2750	C	ARG A		17.393	39.967	14.557	1.00 21.56
MOTA						39.606	13.875	1.00 20.49
MOTA	2751	0	ARG A		16.386			
ATOM	2752	CB	ARG A		17.909	38.835	16.748	1.00 23.44
MOTA	2753	CG	ARG A	408	18.670	37.724	17.479	1.00 25.61
MOTA	2754	CD	ARG A	408	18.838	37.994	18.973	1.00 28.14
MOTA	2755	NE	ARG A	408	17.843	37.328	19.814	1.00 31.17
MOTA	2756	CZ	ARG A		16.567	37.679	19.887	1.00 32.24
	2757		ARG A		16.127	38.693	19.163	1.00 35.70
ATOM					15.735	37.029	20.687	1.00 31.13
ATOM	2758		ARG A					1.00 21.10
MOTA	2759	И	ALA A		17.750	41.241	14.694	
ATOM	2760	CA	ALA A	409	16.978	42.329	14.056	1.00 22.43
MOTA	2761	C	ALA A	409	16.785	42.050	12.571	1.00 22.80
MOTA	2762	0	ALA A	409	15.646	42.177	12.034	1.00 24.04
ATOM	2763	CB	ALA A	409	17.689	43.664	14.247	1.00 20.85
ATOM	2764	N	ARG A		17.858	41.664	11.889	1.00 23.89
ATOM	2765	CA	ARG A		17.770	41.374	10.445	1.00 25.07
			ARG A		17.639	39.888	10.119	1.00 24.26
MOTA	2766	C						
MOTA	2767	0	ARG A				8.956	
MOTA	2768	CB	ARG A		18.987	41.949	9.724	1.00 26.83
ATOM	2769	CG	ARG A	410	19.025	43.464	9.700	1.00 29.89
MOTA	2770	CD	ARG A	410	19.326	43.944	8.295	1.00 32.69
MOTA	2771	NE	ARG A	410	20.590	44.664	8.208	1.00 33.51
ATOM	2772	CZ	ARG A		21.182	44.979	7.062	1.00 34.58
			ARG A		20.626	44.631	5.907	1.00 33.99
MOTA	2773						7.068	1.00 35.27
MOTA	2774		ARG A		22.328			
MOTA	2775	N	LYS A	411	17.223	39.091	11.097	1.00 22.77
MOTA	2776	CA	LYS A		17.061	37.630	10.891	1.00 22.97
MOTA	2777	С	LYS A	411	18.227	37.031	10.104	1.00 21.80
MOTA	2778	0	LYS A		18.015	36.309	9.081	1.00 20.39
MOTA	2779	СВ	LYS A		15.761	37.335	10.138	1.00 23.53
		CG	LYS A		14.491	37.686	10.886	1.00 27.80
MOTA	2780							1.00 30.25
MOTA	2781	CD	LYS A		13.270	37.188	10.121	
MOTA	2782	CE	LYS A		13.337		9.890	1.00 31.18
MOTA	2783	NZ	LYS A		12.153	35.163	9.142	1.00 34.08
ATOM	2784	N .	ARG A		19.449	37.290	10.541	1.00 19.85
MOTA	2785	CA	ARG A	412	20.607	36.748	9.815	1.00 18.29
ATOM	2786	С	ARG A		21.789	36.505	10.736	1.00 18.54
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MOTA	2787	0	ARG A	412	21.911	37.137	11.837	1.00 18.56
ATOM	2788	CB	ARG A	412	21.019	37.714	8.703	1.00 18.72
ATOM	2789.	CG	ARG A	412	21.571	39.027	9.239	1.00 18.66
MOTA	2790	CD	ARG A	412	21.941	39.988	8.127	1.00 18.34
ATOM	2791	NE	ARG A		22.560	41.196	8.662	1.00 19.28
ATOM	2792	CZ	ARG A	412	23.082	42.163	7.916	1.00 20.03
MOTA	2793	NH1	ARG A	412	23.059	42.067	6.591	1.00 19.36
		NH2	ARG A		23.635	43.219	8.496	1.00 19.27
MOTA	2794							
MOTA	2795	N	ILE A	413	22.668	35.606	10.317	1.00 17.01
MOTA	2796	CA	ILE A	413	23.865	35.285	11.103	1.00 16.43
			ILE A		25.103	35.576	10.266	1.00 16.20
MOTA	2797	С						
ATOM	2798	0	ILE A	413	25.213	35.125	9.084	1.00 17.17
ATOM	2799	CB	ILE A	413	23.855	33.808	11.533	1.00 16.02
	2800	CG1	ILE A		22.667	33.562	12.469	1.00 13.92
MOTA								
ATOM	2801	CG2	ILE A	413	25.168	33.458	12.218	1.00 15.95
ATOM	2802	CD1	ILE A	413	22.482	32.130	12.862	1.00 14.89
ATOM	2803	N	GLY A	414	26.028	36.332	10.841	1.00 15.43
								1.00 14.42
ATOM	2804	CA	GLY A		27.243	36.679	10.132	
MOTA	2805	С	GLY A	414	28.463	35.899	10.585	1.00 14.91
ATOM	2806	0	GLY A	414	28.569	35.463	11.779	1.00 12.74
	2807		PHE A		29.392	35.709	9.656	1.00 12.70
ATOM		N						
MOTA	2808	CA	PHE A		30.638	34.977	9.932	1.00 14.84
MOTA	2809	С	PHE A	415	31.823	35.766	9.403	1.00 15.05
MOTA	2810	0	PHE A		31.761	36.376	8.291	1.00 17.34
ATOM	2811	CB	PHE A		30.613	33.599	9.256	1.00 13.57
ATOM	2812	CG	PHE A	415	29.628	32.640	9.860	1.00 13.35
MOTA	2813	CD1	PHE A	415	30.034	31.710	10.820	1.00 14.56
					28.296	32.660	9.472	1.00 11.54
MOTA	2814	CD2	PHE A					
MOTA	2815	CE1	PHE A	415	29.117	30.809	11.383	1.00 13.74
MOTA	2816	CE2	PHE A	415	27.373	31.768	10.027	1.00 12.67
		CZ	PHE A		27.787	30.839	10.985	1.00 13.15
MOTA	2817							
MOTA	2818	N	ALA A	416	32.895	35.779	10.178	1.00 15.11
ATOM	2819	CA	ALA A	416	34.135	36.470	9.786	1.00 14.57
ATOM	2820	C	ALA A		35.248	35.738	10.515	1.00 14.48
MOTA	2821	0	ALA A	416	35.027	35.186	11.639	1.00 12.56
ATOM	2822	CB	ALA A	416	34.095	37.935	10.208	1.00 11.46
ATOM	2823	N	VAL A		36.425	35.692	9.906	1.00 14.71
			VAL A		37.569	35.011	10.528	1.00 16.80
MOTA	2824	CA						
MOTA	2825	С	VAL A	417	37.835	35.634	11.892	1.00 18.08
ATOM	2826	0	VAL A	417	37.922	36.901	12.033	1.00 17.13
ATOM	2827	CB	VAL A		38.824	35.126	9.642	1.00 17.67
MOTA	2828	CGI	VAL A	417	40.022	34.486	10.333	1.00 16.83
MOTA	2829	CG2	VAL A	417	38.561		8.301	1.00 18.32
ATOM	2830	N	SER A		37.953	34.785	12.905	1.00 17.31
			SER A		38.201	35.271	14.272	1.00 17.62
MOTA	2831	CA						
MOTA	2832	C	SER A	418	39.637	35.712	14.455	1.00 18.36
ATOM	2833	0	SER A	418	40.591	35.038	13.963	1.00 19.44
ATOM	2834	CB	SER A		37.882	34.182	15.295	1.00 18.09
								1.00 17.42
ATOM	2835	OG	SER A		38.228	34.617	16.599	
MOTA	2836	N	ALA A	419	39.821	36.827	15.150	1.00 17.60
MOTA	2837	CA	ALA A		41.175	37.335	15.410	1.00 18.46
								1.00 19.09
MOTA	2838	C	ALA A		41.877	36.423	16.423	
ATOM	2839	Ō	ALA A	419	43.117	36.553	16.649	1.00 19.60
ATOM	2840	CB	ALA A		41.106	38.772	15.943	1.00 17.70
					41.132	35.500	17.032	1.00 19.36
MOTA	2841	N	CYS A					
MOTA	2842	CA	CYS A	420	41.736	34.575	18.029	1.00 20.89
MOTA	2843	C	CYS A	420	41.677	33.105	17.624	1.00 19.60
		Õ	CYS A		41.805	32.202	18.501	1.00 22.74
MOTA	2844							
MOTA	2845	CB	CYS A		41.064	34.734	19.410	1.00 21.69
MOTA	2846	SG	CYS A	420	39.353	34.096	19.526	1.00 25.02
MOTA	2847	N	HIS A		41.495	32.814	16.342	1.00 17.86
					41.435		15.933	1.00 17.71
ATOM	2848	CA	HIS A	42T	41.433	31.393	17.333	1.00 1/./1

MOTA	2849	С	HIS A	421	42.834	30.798	15.799	1.00 17.18
ATOM	2850	0	HIS A	421	43.801	31.495	15.356	1.00 14.17
ATOM	2851	CB	HIS A	421	40.641	31.236	14.625	1.00 18.65
MOTA	2852	CG	HIS A	421	41.433	31.504	13.381	1.00 18.77
ATOM	2853	ND1	HIS A		42.114	30.514	12.705	1.00 18.84
ATOM	2854		HIS A		41.631	32.645	12.678	1.00 18.73
ATOM	2855		HIS A		42.695	31.032	11.637	1.00 17.98
ATOM	2856		HIS A		42.418	32.323	11.597	1.00 20.03
ATOM	2857	N	VAL A		42.965	29.533	16.194	1.00 16.96
		CA	VAL A		44.260	28.816	16.132	1.00 16.89
ATOM	2858		VAL A		44.571	28.334	14.719	1.00 17.53
ATOM	2859	C			43.678	27.764	14.021	1.00 17.13
ATOM	2860	0	VAL A		44.257	27.788	17.061	1.00 16.92
ATOM	2861	CB	VAL A		45.632	26.938	17.063	1.00 15.15
ATOM	2862		VAL A			28.004	18.479	1.00 19.33
MOTA	2863	-	VAL A		43.850		14.291	1.00 16.64
ATOM	2864	N	HIS A		45.815	28.531	12.940	1.00 16.92
ATOM	2865	CA	HIS A		46.264	28.112		1.00 10.92
ATOM	2866	С	HIS A		47.792	28.038	12.906	-
MOTA	2867	0	HIS A		48.461	28.105	13.981	1.00 17.20 1.00 15.85
MOTA	2868	CB	HIS A		45.755	29.111	11.889	
MOTA	2869	CG	HIS A		46.242	30.512	12.096	1.00 18.62
ATOM	2870				47.390	30.998	11.504	1.00 19.80
MOTA	2871		HIS A		45.758	31.522	12.857	1.00 17.42
MOTA	2872	CE1	HIS A	423	47.590	32.245	11.892	1.00 18.22
ATOM	2873	NE2	HIS A		46.615	32.586	12.714	1.00 18.53
MOTA	2874	N	ASP A	424	48.360	27.869	11.714	1.00 18.00
MOTA	2875	CA	ASP A	424	49.836	27.817	11.556	1.00 17.75
MOTA	2876	С	ASP A	424	50.194	28.804	10.453	1.00 18.36
MOTA	2877	0	ASP A	424	49.294	29.527	9.935	1.00 20.02
MOTA	2878	СВ	ASP A	424	50.305	26.396	11.206	1.00 18.00
ATOM	2879	ĊĠ	ASP A		49.545	25.791	10.037	1.00 19.08
ATOM	2880	OD1	ASP A		49.110	24.623	10.149	1.00 18.99
ATOM	2881	OD2	ASP A		49.390	26.473	9.003	1.00 20.46
ATOM	2882	N	GLU A		51.459	28.877	10.063	1.00 17.55
MOTA	2883	CA	GLU A		51.813	29.853	9.015	1.00 18.77
ATOM	2884	C	GLU A		51.497	29.379	7.601	1.00 16.95
ATOM	2885	ō	GLU A		51.724	30.131	6.613	1.00 17.24
ATOM	2886	CB	GLU A		53.289	30.239	9.112	1.00 18.65
ATOM	2887	CG	GLU A		54.254	29.150	8.714	1.00 20.84
MOTA	2888	CD	GLU A		55.632	29.697	8.381	1.00 21.89
MOTA	2889	OE1	GLU A		56.481	28.901	7.936	1.00 22.61
MOTA	2890	OE2	GLU A		55.867	30.920	8.559	1.00 22.65
ATOM	2891	N	PHE A		50.955	28.171	7.476	1.00 14.60
MOTA	2892	CA	PHE A		50.619	27.606	6.150	1.00 13.51
ATOM	2893	C	PHE A		49.157	27.767	5.763	1.00 15.14
MOTA	2894	Õ	PHE A		48.826	27.822	4.540	1.00 16.10
ATOM	2895	CB	PHE A		51.001	26.127	6.109	1.00 14.53
ATOM	2896	CG	PHE A		52.452	25.877	6.400	1.00 14.20
	2897		PHE A		53.433	26.244	5.482	1.00 13.59
ATOM	2898		PHE A		52.841	25.298	7.606	1.00 14.11
ATOM			PHE A		54.787	26.040	5.762	1.00 14.83
MOTA	2899		PHE A		54.192	25.087	7.897	1.00 15.49
MOTA	2900				55.167	25.460	6.969	1.00 14.08
MOTA	2901	CZ	PHE A		48.269	27.827	6.752	1.00 13.77
ATOM	2902	N	ARG A		46.824	27.985	6.469	1.00 14.89
ATOM	2903	CA	ARG A		46.130	28.695	7.615	1.00 15.43
MOTA	2904	C	ARG A		46.630	28.710	8.781	1.00 14.58
MOTA	2905	0	ARG A				6.301	1.00 15.33
MOTA	2906	CB	ARG A		46.132	26.632	5.707	1.00 16.84
MOTA	2907	CG	ARG A		46.959	25.518		1.00 17.68
MOTA	2908	CD	ARG A		46.645	24.234	6.477	1.00 16.69
MOTA	2909	NE	ARG A	42/	45.994	23.230	5.655	1.00 15.45
MOTA	2910	CZ	ARG A	427	45.701	21.998	6.062	2.00 20.00

ATOM	2911	NH1	ARG A	427	45.114	21.159	5.224	1.00 14.20
ATOM	2912	NH2	ARG A	427	45.981	21.603	7.296	1.00 13.31
ATOM	2913	N	THR A		44.976	29.269	7.317	1.00 15.28
ATOM	2914	CA	THR A		44.180	29.967	8.336	1.00 17.94
ATOM	2915	C	THR A		42.731	29.650	8.041	1.00 16.25
ATOM	2916	o	THR A		42.400	29.165	6.923	1.00 14.77
		CB	THR A		44.353	31.503	8.249	1.00 18.18
ATOM	2917				44.043	31.942	6.921	1.00 20.24
ATOM	2918	OG1	THR A					1.00 19.84
MOTA	2919	CG2	THR A		45.773	31.901	8.583	1.00 15.84
MOTA	2920	N	ALA A		41.860	29.901	9.009	
MOTA	2921	CA	ALA A		40.423	29.677	8.803	1.00 16.03
ATOM	2922	C.	ALA A		40.048	30.739	7.775	1.00 15.66
ATOM	2923	0	ALA A	429	40.808	31.738	7.574	1.00 14.51
ATOM	2924	CB	ALA A	429	39.656	29.898	10.105	1.00 17.08
ATOM	2925	N	ALA A	430	38.920	30.575	7.107	1.00 14.04
ATOM	2926	CA	ALA A	430	38.556	31.576	6.100	1.00 13.71
ATOM	2927	С	ALA A	430	37.067	31.706	5.883	1.00 11.98
ATOM	2928	0	ALA A	430	36.271	30.754	6.166	1.00 12.33
ATOM	2929	СВ	ALA A	430	39.251	31.246	4.762	1.00 12.27
MOTA	2930	N	VAL A		36.671	32.874	5.396	1.00 11.01
MOTA	2931	CA	VAL A		35.260	33.149	5.076	1.00 13.39
ATOM	2932	C	VAL A		35.344	33.773	3.697	1.00 15.69
ATOM	2933	Ö	VAL A		35.857	34.926	3.533	1.00 17.86
ATOM	2934	СВ	VAL F		34.624	34.145	6.056	1.00 11.50
ATOM	2935	CG1	VAL A		33.148	34.294	5.737	1.00 10.61
	2936	CG2	VAL A		34.818	33.659	7.494	1.00 10.71
MOTA		. N	GLU A		34.874	33.048	2.694	1.00 16.74
MOTA	-		GLU A		34.969	33.544	1.320	1.00 18.65
ATOM	2938	CA				33.414	0.530	1.00 18.40
MOTA	2939	C	GLU A		33.681	32.567	0.852	1.00 16.81
MOTA	2940	0	GLU A		32.794			1.00 10.01
MOTA	2941	СВ	GLU A		36.097	32.796	0.607	
MOTA	2942	CG	GLU A		37.460	33.031	1.241	1.00 24.66
MOTA	2943	CD	GLU A		38.466	31.930	0.935	1.00 27.80
MOTA	2944	OE1	GLU A		39.681	32.196	1.051	1.00 30.84
MOTA	2945	OE2	GLU A		38.049	30.799	0.595	1.00 28.87
MOTA	2946	N	GLY A		33.574	34.243	-0.504	1.00 18.95
MOTA	2947	CA	GLY A	433	32.408	34.244	-1.363	1.00 19.36
MOTA	2948	С	GLY A	433	32.504	35.385	-2.359	1.00 19.59
MOTA	2949	0	GLY A	433	33.489	36.173	-2.328	1.00 18.33
MOTA	2950	N	PRO A	434	31.511	35.539	-3.243	1.00 19.47
MOTA	2951	CA	PRO A	434	30.345	34.655	-3.285	1.00 19.72
ATOM	2952	С	PRO A	434	30.485	33.589	-4.353	1.00 19.98
MOTA	2953	0	PRO A	434	31.382	33.674	-5.235	1.00 22.24
MOTA	2954	CB	PRO A		29.215	35.619	-3.595	1.00 19.80
ATOM	2955	CG	PRO A		29.869	36.517	-4.616	1.00 19.70
ATOM	2956	CD	PRO A		31.261	36.770	-4.018	1.00 19.73
MOTA	2957	N	PHE A		29.624	32.583	-4.290	1.00 21.45
ATOM	2958	CA	PHE A		29.619	31.502	-5.292	1.00 22.31
MOTA	2959	C	PHE 2		28.217	31.513	~5.872	1.00 24.39
ATOM	2960	ō	PHE 2		27.207	31.636	-5.110	1.00 24.58
ATOM	2961	СВ	PHE A		29.924	30.155	-4.636	1.00 22.02
	2962	CG	PHE 2		31.215	30.141	-3.876	1.00 20.80
MOTA	2963		PHE I		31.232	30.392	-2.507	1.00 20.70
MOTA					32.424	29.945	-4.542	1.00 21.70
MOTA	2964		PHE A		32.432	30.451	-1.809	1.00 20.27
MOTA	2965		PHE A					1.00 20.27
ATOM	2966		PHE A		33.634	30.003	-3.853	1.00 21.53
MOTA	2967	CZ	PHE A		33.637	30.259	-2.481	1.00 27.02
ATOM	2968	N	VAL A		28.117	31.396	-7.192	
MOTA	2969	CA	VAL I		26.802	31.438	-7.872	1.00 29.79
MOTA	2970	С	VAL A		26.526	30.219	-8.739	1.00 32.85
MOTA	2971	0	VAL A		25.434	30.120	-9.376	1.00 33.81
MOTA	2972	CB	VAL 2	436	26.702	32.677	-8.787	1.00 28.98

MOTA	2973	CG1	VAL	A	436	26.999	33.944	-7.996	1.00 29.00
MOTA	2974	CG2	VAL	A	436	27.678	32.537	-9.947	1.00 28.49
MOTA	2975	N	THR			27.473	29.292	-8.795	1.00 36.05
ATOM	2976	ÇA	THR			27.305	28.089	-9.638	1.00 39.30
	2977	С	THR			26.582	26.979	-8.870	1.00 41.99
ATOM	2978	Ō	THR			26.604	25.775	-9.276	1.00 41.77
ATOM	2979	CB	THR			28.690		-10.123	1.00 39.02
MOTA	2980	OG1	THR			28.552		-11.408	1.00 42.51
ATOM	2981	CG2	THR			29.280	26.578	-9.156	1.00 38.10
ATOM		N CGZ	LEU			25.908	27.368	-7.794	1.00 38.10
	2982		_					-6.901	1.00 49.22
MOTA	2983	CA	LEU			25.199	26.417		
ATOM	2984	C	LEU			23.753	26.016	-7.165	1.00 50.49
MOTA	2985	0	LEU			22.869	26.878	-7.466	1.00 51.99
MOTA	2986	СВ	LEU			25.276	26.944	-5.473	1.00 50.30
ATOM	2987	CG	LEU			26.027	28.269	-5.358	1.00 50.73
MOTA	2988		LEU			25.108	29.457	-5.584	1.00 50.27
ATOM	2989		LEU			26.629	28.328	-4.001	1.00 51.67
ATOM	2990	N	ASP			23.505	24.715	-7.037	1.00 52.67
ATOM	2991	CA	ASP			22.149	24.128	-7.172	1.00 55.74
MOTA	2992	С	ASP			21.690	24.224	-5.722	1.00 56.96
MOTA	2993	0	ASP			21.757	23.221	-4.945	1.00 57.33
MOTA	2994	CB	ASP			22.240	22.657	-7.586	1.00 56.39
ATOM	2995	CG	ASP			20.879	21.993	-7.695	1.00 57.68
MOTA	2996	OD1				20.046	22.178	-6.781	1.00 57.75
ATOM	2997	OD2	ASP	A	439	20.645	21.274	-8.692	1.00 58.18
MOTA	2998	N	MET			21.233	25.407	-5.337	1.00 58.71
ATOM	2999	CA	MET	A	440	20.841	25.656	-3.944	1.00 60.87
ATOM	3000	C	MET	A	440	19.435	26.215	-3.713	1.00 62.52
MOTA	3001	0	MET	Α	440	19.247	27.451	-3.489	1.00 63.93
MOTA	3002	CB	MET	A	440	21.916	26.569	-3.346	1.00 60.48
MOTA	3003	CG	MET	Α	440	21.523	27.456	-2.201	1.00 60.72
ATOM	3004	SD	MET .	Α	440	22.755	28.755	-2.086	1.00 59.28
ATOM	3005	CE	MET .	Α	440	22.367	29.689	-3.543	1.00 59.46
ATOM	3006	N	GLU .	Α	441	18.435	25.343	-3.765	1.00 63.61
MOTA	3007	CA	GLU .	A	441	17.042	25.774	-3.514	1.00 65.54
ATOM	3008	C	GLU .	A	441	16.356	24.847	~2.518	1.00 64.49
ATOM	3009	0	GLU .	A	441	15.998	25.285	-1.375	1.00 65.36
MOTA	3010	CB	GLU .	A	441	16.229	25.847	-4.815	1.00 67.99
MOTA	3011	CG	GLU .	A	441	16.500	24.745	-5.822	1.00 70.98
ATOM	3012	CD	GLU .	Α	441	17.353	25.228	-6.981	1.00 72.23
ATOM	3013	OE1	GLU .	A	441	18.507	25.646	-6.742	1.00 73.24
ATOM	3014	OE2	GLU .			16.867	25.194	-8.132	1.00 73.30
MOTA	3015	N	ASP .	A	442	16.170	23.585	-2.896	1.00 61.29
ATOM	3016	CA	ASP .			15.519	22.616	-1.986	1.00 58.37
ATOM	3017	C .	ASP .			16.504	21.966	-1.018	1.00 55.47
ATOM	3018	0	ASP .	Α	442	16.615	20.704	-0.950	1.00 54.59
MOTA	3019	СВ	ASP :			14.800	21.530	-2.785	1.00 59.93
MOTA	3020	CG	ASP .			13.298	21.616	-2.646	1.00 60.90
ATOM	3021		ASP .			12.689	22.478	-3.312	1.00 61.34
ATOM	3022		ASP .			12.729	20.832	-1.854	1.00 61.81
ATOM	3023	N	CYS .			17.207	22.790	-0.252	1.00 51.31
MOTA	3024	CA	CYS .			18.200	22.281	0.713	1.00 47.79
ATOM	3025	C	CYS			17.635	22.156	2.121	1.00 46.40
MOTA	3026	ō	CYS			18.168	21.373	2.965	1.00 44.04
MOTA	3027	СВ	CYS			19.421	23.198	0.713	1.00 48.61
ATOM	3028	SG	CYS			20.176	23.339	-0.939	1.00 46.95
MOTA	3029	N	GLY :			16.566	22.895	2.395	1.00 45.40
ATOM	3030	CA	GLY :			15.953	22.846	3.709	1.00 45.06
ATOM	3031	C	GLY A			15.011	21.673	3.899	1.00 45.25
ATOM	3032	0	GLY :			14.271	21.264	2.952	1.00 44.97
ATOM	3033	И	TYR 3			15.018	21.109	5.101	1.00 44.97
ATOM	3034	CA	TYR 2			14.140	19.968	5.421	1.00 44.48
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MOTA	3035	С	TYR	A	445		12.778	20.467	5.882	1.00 45.23
MOTA	3036	0	TYR				12.662		6.530	1.00 44.57
MOTA	3037	CB	TYR	A	445		14.801	19.172	6.531	1.00 43.11
MOTA	3038	CG	TYR				13.918		6.871	1.00 42.75
MOTA	3039	CD1	TYR				13.846		6.010	1.00 42.58
MOTA	3040	CD2	TYR				13.170		8.049	1.00 42.27
MOTA	3041	CE1	TYR	Α	445		13.042	15.820	6.327	1.00 41.99
MOTA	3042	CE2	TYR	Α	445		12.358	16.917	8.360	1.00 43.20
MOTA	3043	CZ	TYR	Α	445		12.289	15.835	7.503	1.00 41.98
MOTA	3044	OH	TYR	Α	445		11.490	14.751	7.810	1.00 20.00
ATOM	3045	N	ASN	A	446	;	11.746	19.699	5.550	1.00 45.69
MOTA	3046	CA	ASN				10.359	20.012	5.947	1.00 48.64
ATOM.	3047.	С	ASN				9.776		6.524	1.00 50.90
MOTA	3048	0	ASN				9.894		5.896	1.00 51.59
ATOM	3049	CB	ASN				9.537		4.738	1.00 48.19
MOTA	3050	CG	ASN				9.975		4.213	1.00 48.18
MOTA	3051		ASN				9.926		4.950	1.00 48.63
MOTA	3052		ASN			;	10.403		2.957	1.00 48.04
MOTA	3053	N	ILE				9.165		7.700	1.00 53.94
MOTA	3054	CA	ILE				8.569		8.388	1.00 55.99
ATOM	3055	C	ILE				7.720		7.463	1.00 57.01
ATOM	3056	0	ILE				7.449		6.318	1.00 58.11
ATOM	3057	CB	ILE				7.699		9.577	1.00 55.86
MOTA	3058	CG1	ILE				8.488	19.086	10.450	1.00 56.28
ATOM	3059	CG2	ILE				7.267		10.406	1.00 56.92
ATOM	3060	CD1	ILE				9.759		11.037	1.00 55.79
MOTA	3061	OXT	ILE		447		7.328	15.666	7.895	1.00 57.55
MOTA	3062	N	SER		1		35.528	15.672	28.238	1.00 37.61
ATOM	3063 3064	CA C	SER SER		1 1		34.172	16.082 16.863	28.590 27.450	1.00 36.72 1.00 34.75
ATOM	3065	0	SER		1		33.508 34.132	17.643	26.742	1.00 34.75
MOTA	3065		SER		1		34.248	16.949	29.848	1.00 30.45
ATOM	3067	CB.	SER		1		33.152	17.865	29.853	1.00 37.77
ATOM ATOM	3068	og N	GLU		2		32.203	16.601	27.257	1.00 40.82
ATOM	3069	CA	GLU		2		31.513	17.216	26.129	1.00 32.80
ATOM	3070	C	GLU		2		30.218	17.216	26.552	1.00 32.80
ATOM	3071	Ö	GLU		2		29.435	17.401	27.348	1.00 31.23
ATOM	3072	CB	GLU		2		31.275		25.027	1.00 33.64
ATOM	3073	CG	GLU		2		31.096	17.096	23.826	1.00 37.41
ATOM	3074	CD	GLU		2		31.076	15.940	22.852	1.00 38.37
ATOM	3075		GLU		2		31.996	15.134	22.983	1.00 39.04
ATOM	3076		GLU		2		30.175	15.798	22.037	1.00 39.43
ATOM	3077	N	VAL		3		9.742	19.344	26.106	1.00 27.98
MOTA	3078	CA	VAL		3		28.367	19.820	26.101	1.00 26.44
MOTA	3079	С	VAL	P	3	2	27.717	19.598	24.735	1.00 26.26
MOTA	3080	0	VAL	P	3		28.371	19.580	23.701	1.00 25.48
MOTA	3081	CB	VAL	P	3	2	28.377	21.311	26.429	1.00 25.89
ATOM	3082	CG1	VAL	P	3	. 2	8.684	21.516	27.911	1.00 27.07
ATOM	3083	CG2	VAL	P	3	2	9.431	22.012	25.594	1.00 23.97
MOTA	3084	N	ASN	P	4	2	6.361	19.591	25.174	1.00 25.89
MOTA	3085	CA	ASN	P	4	2	25.421	19.254	24.075	1.00 26.64
MOTA	3086	C	ASN	P	4	2	4.027	19.825	24.452	1.00 26.87
MOTA	3087	0	ASN	P	4	2	3.116	19.163	25.077	1.00 27.10
	3088		ASN		4		5.349	17.766	23.876	1.00 27.95
	3089		ASN		4		6.498	17.245	22.971	1.00 29.39
MOTA	3090		ASN		4		6.499	17.409	21.723	1.00 31.90
	3091		ASN		4		7.489	16.617	23.603	1.00 31.97
		N	STA		5		4.115	21.101	24.323	1.00 25.26
	3093	CA	STA		5		2.965	21.865	24.929	1.00 25,83
	3094	CB	STA		5		3.683	22.681	26.021	1.00 27.28
	3095	CG	STA		5		4.378	22.057	27.197	1.00 28.07
MOTA	3096	CD1	STA	P	5	2	5.002	23.077	28.182	1.00 27.46

ATOM	3097	CD2	STA	P	5	23.280	21.130	27.828	1.00 25.47
ATOM	3098	CH	STA	P	5	22.223	22.851	23.940	1.00 25.86
					5	23.028	23.679	23.298	1.00 25.23
ATOM	3099	OH	STA						
ATOM	3100	CM	STA		5	21.372	21.980	23.048	1.00 27.11
ATOM	3101	С	STA	P	5	20.420	21.340	24.125	1.00 27.81
ATOM	3102	0	STA	P	5	20.241	20.065	24.095	1.00 25.70
ATOM	3103	N	VAL	Р	6	19.339	22.479	23.764	1.00 26.04
ATOM	3104	CA	VAL		6	18.037	21.953	24.156	1.00 27.12
	3105	C	VAL		6	17.496	20.965	23.121	1.00 27.36
MOTA									
MOTA	3106	0	VAL		6	17.795	21.029	21.936	1.00 26.97
MOTA	3107	CB	VAL	P	6	17.073	23.130	24.312	1.00 27.18
ATOM	3108	CG1	VAL	P	6	16.433	23.463	22.965	1.00 26.70
MOTA	3109	CG2	VAL	P	6	15.985	22.781	25.311	1.00 28.74
MOTA	3110	N	ALA	P	7	16.702	19.998	23.617	1.00 28.68
ATOM	3111	CA	ALA		7	16.158	18.986	22.720	1.00 32.14
MOTA	3112	C	ALA		7	14.774	19.377	22.197	1.00 32.99
									1.00 32.08
MOTA	3113	0	ALA		7	14.040	20.149	22.801	
ATOM	3114	CB	ALA		7	16.072	17.666	23.489	1.00 31.38
MOTA	3115	N	GLU	P	8	14.443	18.843	21.007	1.00 36.10
MOTA	3116	CA	GLU	P	8	13.144	19.143	20.418	1.00 39.90
MOTA	3117	С	GLU	P	8	12.012	18.425	21.158	1.00 41.72
ATOM	3118	0	GLU		8	12.189	17.359	21.733	1.00 41.52
ATOM	3119	СВ	GLU		8	13.172	18.705	18.952	1.00 39.88
					8	14.037	19.626	18.090	1.00 41.02
MOTA	3120	CG	GLU						
MOTA	3121	CD	GLU		8	13.896	19.235	16.637	1.00 41.83
ATOM	3122		GLU		8	14.911	19.052	15.979	1.00 41.60
ATOM	3123	OE2	GLU	P	8	12.765	19.124	16.169	1.00 41.88
ATOM	3124	N	PHE	P	9	10.811	18.986	21.162	1.00 45.62
MOTA	3125	CA	PHE	P	9	9.677	18.356	21.865	1.00 49.63
ATOM	3126	C		P	9	9.382	16.960	21.337	1.00 50.61
ATOM	3127	ō	PHE		9	9.156	16.839	20.116	
					9	8.451	19.245	21.670	1.00 50.65
ATOM	3128	CB		P					
MOTA	3129	CG	PHE		9	8.607	20.501	22.499	1.00 52.48
MOTA	3130	CD1	PHE	P	9	8.278	20.493	23.849	1.00 52.80
ATOM	3131	CD2	PHE	P	9	9.073	21.659	21.899	1.00 53.12
MOTA	3132	CEl	PHE	P	9	8.420	21.651	24.600	1.00 53.74
ATOM	3133	CE2	PHE	P	9	9.215	22.817	22.659	1.00 53.61
MOTA	3134	CZ	PHE	P	9	8.890	22.817	24.010	1.00 54.24
ATOM	31:35			P	9	9.383	16.011	22,152	1.00 51.56
ATOM	3136	OH2	TIP		2	37.673	4.149	14.933	1.00 18.73
							19.019	28.545	1.00 20.36
MOTA	3137	OH2	TIP		3	37.999			
MOTA	3138		TIP		12	46.550	23.555	9.446	1.00 16.05
MOTA	3139	OH2	TIP	С	14	18.354			1.00 14.14
ATOM	3140	он2	TIP	C	15	33.073	10.884	15.835	1.00 14.30
ATOM	3141	OH2	TIP	С	16	15.032	34.698	31.070	1.00 11.96
MOTA	3142	OH2	TIP	C	17	7.170	35.908	33.277	1.00 16.70
MOTA	3143		TIP		19	16.624	32.704	28.166	1.00 15.10
ATOM	3144		TIP		20	35.078	42.552	29.609	1.00 19.72
						40.457	30.360	27.755	1.00 16.31
MOTA	3145		TIP		21			9.725	1.00 20.11
MOTA	3146		TIP		22	52.263	20.430		
MOTA	3147	OH2	TIP	C	23	20.720	20.412	14.822	1.00 12.68
MOTA	3148	OH2	TIP	C	24	33.413	15.317	~5.393	1.00 15.90
ATOM	3149	OH2	TIP	С	25	38.275	25.072	23.469	1.00 13.40
MOTA	3150	OH2	TIP	С	27	16.591	21.729	7.186	1.00 19.86
MOTA	3151		TIP		28	21.798	19.346	19.780	1.00 14.31
	3152		TIP		29	17.533	34.724	25.177	1.00 16.69
MOTA									1.00 19.19
MOTA	3153		TIP		30	29.162	27.768	25.821	
MOTA	3154		TIP		31	40.631	28.021	16.946	1.00 14.53
MOTA	3155	OH2	TIP	С	32	32.428	32.415	17.998	1.00 10.42
MOTA	3156	OH2	TIP	С	33	11.884	34.798	21.161	1.00 23.00
ATOM	3157		TIP		34	27.837	25.769	-5.173	1.00 33.18
MOTA	3158		TIP		35	12.372	31.279	28.339	1.00 16.96

MOTA	3159	OH2	TIP	С	36	39.263	28.648	25.755	1.00	9.84
ATOM	3160	OH2	TIP	С	40	38.924	30.840	30.171	1.00	13.35
MOTA	3161	OH2	TIP	C	41	18.085	18.989	18.858	1.00	16.60
ATOM	3162	OH2	TIP		42	7.300	35.692	30.168	-	19.22
								30.405		18.32
MOTA	3163	OH2	TIP		43	14.250	32.017			
MOTA	3164	OH2	TIP		44	37.440	22.761	1.333		23.96
MOTA	3165	OH2	TIP	С	45	29.932	39.949	32.969		22.64
ATOM	3166	OH2	TIP	С	46	29.433	17.902	20.935	1.00	16.15
ATOM	3167	OH2	TIP		47	53.536	22.468	21.774	1.00	21.62
ATOM	3168	OH2	TIP		48	40.180	15.699	-0.272		12.15
					49	14.955	25.973	25.745		11.98
MOTA	3169	OH2					_			
MOTA	3170	OH2	TIP		50	38.595	6.527	3.885		23.66
ATOM	3171	OH2	TIP		51	48.551	24.793	17.574		18.30
MOTA	3172	OH2	TIP	С	52	20.747	27.407	17.869	1.00	8.25
ATOM	3173	OH2	TIP	С	53	26.489	18.730	30.746	1.00	26.59
MOTA	3174	OH2	TIP	С	54	38.723	11.162	19.249	1.00	11.49
ATOM	3175	OH2	TIP		55	33.881	26.191	31.382	1.00	19.21
ATOM	3176		TIP		56	13.322	31.213	40.027	1.00	15.61
			TIP		57	19.497	16.134	41.439		26.82
MOTA	3177					38.469	37.062	5.695		23.10
MOTA	3178	OH2	TIP		58					
MOTA	3179	он2	TIP		59	45.575	15.894	3.122		18.45
MOTA	3180	OH2	TIP	С	60	39.615	25.333	-1.743		20.09
MOTA	3181	OH2	TIP	С	61	32.158	37.928	32.431	1.00	12.17
MOTA	3182	OH2	TIP	С	62	46.793	19.609	22.823	1.00	19.81
ATOM	3183	OH2	TIP	С	63	24.847	37.031	-0.659	1.00	29.98
ATOM	3184		TIP		64	45.957	18.715	3.836		18.88
			TIP		65	36.189	33.100	17.653		10.63
MOTA	3185						25.020	24.150		28.40
MOTA	3186		TIP		66	31.177				
MOTA	3187		TIP		67	46.181	23.210	18.466		20.41
MOTA	3188	-	TIP		68	21.756	10.923	7.943		22.80
MOTA	3189	OH2	TIP	С	69	12.936	36.695	30.481		17.63
ATOM	3190	OH2	TIP	С	70	33.713	44.843	8.382	1.00	30.49
ATOM	3191	OH2	TIP	С	71	21.051	41.550	39.982	1.00	31.15
ATOM	3192		TIP		72	26.815	38.732	3.198	1.00	22.61
ATOM	3193	OH2	TIP		73	41.656	24.820	21.177		19.69
		OH2			74	25.521	30.139	47.617		31.08
MOTA	3194		TIP				46.537	15.336		29.67
MOTA	3195	OH2	TIP		75	20.497				
ATOM	3196	OH2	TIP		76	7.708	28.422	41.027		26.00
MOTA	3197	OH2	TIP	C	77	25.650	18.585	27.821		17.30
MOTA	3198	OH2	TIP	С	78	35.124	16.582	21.374		15.44
ATOM	3199	OH2	TIP	С	79	16.806	29.258	45.952	1.00	22.64
MOTA	3200	OH2	TIP	С	80	29.365	7.305	14.767	1.00	28.00
ATOM	3201		TIP		81	36.259	9.577	-0.018	1.00	36.72
ATOM	3202		TIP	-	82	5.598	37.375	35.367	1.00	29.64
	3203		TIP		83	14.256	22.267	9.863		20.30
MOTA								41.318		35.70
ATOM	3204		TIP		84	34.533	14.826			22.15
MOTA	3205		TIP		85	14.253	38.931	17.469		
MOTA	3206	OH2	TIP	С	86	40.762	43.633	8.075		32.27
MOTA	3207	OH2	TIP	С	87	20.139	38.471	47.202		19.79
ATOM	3208	OH2	TIP	С	88	49.003	25.388	14.809		16.95
ATOM	3209	OH2	TIP	С	89	48.376	21.580	21.346	1.00	26.51
ATOM	3210		TIP		90	38.281	15.314	27.561	1.00	34.16
ATOM	3211		TIP		91	8.631	39.984	34.095		41.37
					92	50.906	23.612	20.744		52.18
MOTA	3212		TIP							24.16
MOTA	3213		TIP		93	53.785	20.060	24.538		
MOTA	3214		TIP		94	24.823	42.619	11.579		21.18
MOTA	3215	OH2	TIP	С	95	25.075	45.083	6.146		38.65
MOTA	3216	OH2	TIP	C	96	40.830	25.584	18.443		18.31
ATOM	3217	OH2	TIP	C	97	43.416	22.239	18.182		19.16
MOTA	3218		TIP		98	13.417	34.174	40.223		31.15
ATOM	3219		TIP		99	33.278	34.940	35.258	1.00	19.39
ATOM	3220		TIP			16.214	11.125	16.638		44.74
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ATOM	3221	OH2	TIP C	101	53.364	20.723	14.579	1.00 34.15
ATOM	3222	OH2	TIP C	102	49.883	22.898	7.975	1.00 17.76
			TIP C		23.025	15.361	39.364	1.00 32.71
ATOM	3223	OH2						<del>-</del>
ATOM	3224	OH2	TIP C	104	9.989	41.920	29.368	1.00 18.54
MOTA	3225	OH2	TIP C	105	40.434	26.276	24.857	1.00 17.36
MOTA	3226	OH2	TIP C	106	20.997	29.964	6.095	1.00 20.90
						47.336	16.035	1.00 24.48
ATOM	3227	OH2	TIP C		27.762			
ATOM	3228	OH2	TIP C	108	49.284	22.771	5.126	1.00 18.73
ATOM	3229	OH2	TIP C	109	48.838	23.239	29.592	1.00 33.97
ATOM	3230	OH2	TIP C	110	28.582	23.099	35.349	1.00 20.25
ATOM	3231	OH2	TIP C		32.528	35.162	39.110	1.00 29.39
								1.00 29.24
ATOM	3232	OH2	TIP C		41.404	21.066	27.696	
MOTA	3233	OH2	TIP C	113	41.566	30.795	24.916	1.00 29.04
ATOM	3234	OH2	TIP C	114	38.888	34.349	4.634	1.00 19.24
ATOM	3235	OH2	TIP C	115	21.524	13.318	6.181	1.00 21.83
ATOM	3236	OH2	TIP C		20.262	44.365	41.166	1.00 51.68
						37.586	7.262	1.00 26.48
MOTA	3237	OH2	TIP C		40.866			
MOTA	3238	OH2	TIP C		24.269	19.013	20.381	1.00 20.56
ATOM	3239	OH2	TIP C	119	14.796	40.366	21.026	1.00 26.21
ATOM	3240	OH2	TIP C	120	40.271	21.968	24.452	1.00 22.99
ATOM	3241	OH2	TIP C		27.256	8.206	3.568	1.00 32.16
					38.453	23.426	21.155	1.00 20.65
ATOM	3242	OH2	TIP C					
ATOM	3243	OH2	TIP C		39.489	30.192	18.787	1.00 19.64
ATOM	3244	OH2	TIP C	124	49.479	24.877	3.120	1.00 15.38
MOTA	3245	OH2	TIP C	125	23.534	17.922	36.838	1.00 21.55
ATOM	3246	OH2	TIP C		24.481	13.568	37.531	1.00 33.00
			TIP C		27.515	37.075	45.132	1.00 32.65
ATOM								
ATOM	3248	OH2	TIP C		20.903	11.530	10.774	1.00 25.13
MOTA	3249	OH2	TIP C	129	16.996	37.117	6.834	1.00 26.72
ATOM	3250	OH2	TIP C	130	42.280	39.848	5.806	1.00 39.08
ATOM-	3251	OH2	TIP C		15.426	37.238	14.643	1.00 27.36
			TIP C		47.740	29.973	16.321	1.00 27.58
ATOM	3252	OH2						
ATOM	3253	OH2	TIP C		52.162	19.864	18.278	1.00 19.10
MOTA	3254	OH2	TIP C	134	47.805	11.416	4.529	1.00 30.40
ATOM	3255	OH2	TIP C	135	20.920	22.905	41.964	1.00 23.80
ATOM	3256	OH2	TIP C		27.784	19.013	-1.506	1.00 28.71
		OH2	TIP C		25.506	36.437	2.115	1.00 19.53
MOTA	3257							1.00 30.54
MOTA	3258	OH2	TIP C		6.347	36.058	44.801	
MOTA	3259	OH2	TIP C		18.428	23.862	8.397	1.00 19.65
MOTA	3260	OH2	TIP C	140	56.631	14.945	24.048	1.00 29.26
ATOM	3261	OH2	TIP C		36.045	33.381	-3.424	1.00 39.63
	3262		TIP C		20.242	14.180	11.802	1.00 31.49
ATOM					8.614	22.301		1.00 30.94
ATOM			TIP C					
MOTA	3264		TIP C		8.697	38.736	31.440	1.00 44.64
MOTA	3265		TIP C		21.002		40.621	1.00 23.34
MOTA	3266	OH2	TIP C	146	36.343	37.533	7.628	1.00 25.43
ATOM	3267		TIP C		13.944	44.970	51.125	1.00 40.01
	3268		TIP C		12.509	22.964	23.735	1.00 33.44
MOTA								1.00 30.50
MOTA	3269		TIP C		32.555	6.398	6.686	
MOTA	3270	OH2	TIP C	150	11.123	30.018	41.695	1.00 29.12
ATOM	3271	OH2	TIP C	151	20.406	19.454	17.419	1.00 26.72
ATOM	3272		TIP C		37.729	21.375	25.750	1.00 27.16
			TIP C		36.922	28.170	33.507	1.00 42.28
ATOM	3273						32.277	1.00 19.72
MOTA	3274		TIP C		13.904	29.766		
ATOM	3275		TIP C		54.556	19.732	11.775	1.00 37.67
MOTA	3276	OH2	TIP C	156	14.999	28.327	48.310	1.00 40.64
ATOM	3277		TIP C		19.001	46.759	12.106	1.00 40.48
MOTA	3278		TIP C		22.361	9.339	13.691	1.00 44.57
					26.097		36.996	1.00 27.61
MOTA	3279		TIP C					1.00 27.01
MOTA	3280		TIP C		51.862	24.669	14.501	
MOTA	3281		TIP C		42.713		38.299	1.00 37.21
ATOM	3282	OH2	TIP C	162	32.074	43.316	6.583	1.00 32.14

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MOTA	3283	OH2 TIP C	163	44.434	22.056	2.693	1.00 44.76
MOTA	3284	OH2 TIP C	164	24.074	33.090	45.770	1.00 26.95
	3285		165	12.289	35.656	48.500	1.00 33.30
MOTA						51.538	1.00 48.93
ATOM	3286		166	19.499	27.253		
MOTA	3287	OH2 TIP C	167	28.896	14.390	20.410	1.00 32.12
MOTA	3288	OH2 TIP C	168	7.799	34.543	25.107	1.00 34.11
			169	41.359	33.697	5.939	1.00 29.72
ATOM	3289					46.449	1.00 37.54
ATOM	3290		170	26.378	23.008		
MOTA	3291	OH2 TIP C	171	10.530	41.770	49.010	1.00 34.66
MOTA	3292	OH2 TIP C	172	41.154	5.586	4.533	1.00 25.18
	3293		173	17.462	11.487	4.521	1.00 46.32
ATOM					39.527	37.113	1.00 36.37
MOTA	3294		174	7.600			
MOTA	3295	OH2 TIP C	175	3.552	23.235	37.583	1.00 39.37
MOTA	3296	OH2 TIP C	176	32.818	21.891	40.191	1.00 36.81
ATOM	3297		177	30.404	26.159	40.588	1.00 38.22
		OH2 TIP C		16.691	29.183	54.400	1.00 39.76
MOTA	3298				47.986	22.417	1.00 32.19
MOTA	3299		179	16.247			
ATOM	3300		180	37.394	44.558	11.594	1.00 39.03
MOTA	3301	OH2 TIP C	181	53.552	27.209	11.822	1.00 47.97
MOTA	3302		182	10.503	32.709	12.025	1.00 38.41
		OH2 TIP C		17.985	14.916	28.259	1.00 36.86
MOTA	3303			25.047	45.446	12.174	1.00 49.92
MOTA	3304		184				
MOTA	3305	OH2 TIP C	185	16.402	15.741	36.532	1.00 40.29
ATOM	3306	OH2 TIP C	186	51.364	22.471	17.335	1.00 28.11
MOTA	3307	OH2 TIP C	187	25.633	28.369	50.282	1.00 42.57
		OH2 TIP C		35.183	14.816	0.037	1.00 36.60
MOTA	3308				26.536	23.386	1.00 44.75
MOTA	3309	OH2 TIP C		8.318			
MOTA	3310	OH2 TIP C		47.893	17.794	24.745	1.00 42.51
ATOM	3311	OH2 TIP C	191	2.728	32.293	36.650	1.00 38.36
ATOM	3312	OH2 TIP C		30.315	9.929	15.860	1.00 39.58
		OH2 TIP C		29.613	40.378	2.225	1.00 41.26
MOTA	3313						1.00 43.60
MOTA	3314	OH2 TIP C		14.241	43.934	16.316	
MOTA	3315	OH2 TIP C	195	48.673	31.215	7.801	1.00 32.67
MOTA	3316	OH2 TIP C	196	10.948	21.963	18.969	1.00 41.87
ATOM	3317	OH2 TIP C		37.378	39.077	3.714	1.00 35.77
				24.488	11.993	21.654	1.00 38.05
ATOM	3318	OH2 TIP C				4.946	1.00 48.02
ATOM	3319	OH2 TIP C		47.986	31.378		•
MOTA	3320	OH2 TIP C		15.373	46.520	15.659	1.00 45.30
MOTA	3321	OH2 TIP C	201	29.464	40.417	40.154	1.00 40.62
ATOM	3322	OH2 TIP C		56.018	18.652	7.189	1.00 43.28
	3323	OH2 TIP C		36.508	17.526	41.765	1.00 61.21
MOTA					36.523	-0.637	1.00 43.56
ATOM	3324	OH2 TIP C		36.132			1.00 47.33
MOTA	3325	OH2 TIP C		9.832		46.230	
MOTA	3326	OH2 TIP C	206	12.086	37.731	18.949	1.00 44.12
ATOM	3327	OH2 TIP C		4.729	26.744	22.711	1.00 40.03
	3328	OH2 TIP C		9.555	36.540	23.357	1.00 46.94
MOTA				23.046	47.732	4.343	1.00 48.13
MOTA	3329	OH2 TIP C					1.00 64.51
ATOM	3330	OH2 TIP C	210	39.932	44.592	5.460	
MOTA	3331	OH2 TIP C	211	17.996	41.071	6.267	1.00 48.35
ATOM	3332	OH2 TIP C		17.866	46.493	17.139	1.00 39.09
		OH2 TIP C		55.520	11.908	17.658	1.00 43.06
ATOM	3333			3.059	35.093	42.826	1.00 38.97
ATOM	3334	OH2 TIP C					
ATOM	3335	OH2 TIP C		31.593	14.910	43.677	1.00 44.01
ATOM	3336	OH2 TIP C	216	33.045	23.673	44.607	1.00 45.50
MOTA	3337	OH2 TIP C		42.870	35.555	7.510	1.00 29.79
		OH2 TIP C		4.112	25.648	42.564	1.00 56.65
MOTA	3338					20.446	1.00 47.85
MOTA	3339	OH2 TIP C			8.547		
ATOM	3340	OH2 TIP C		~0.925		41.173	1.00 36.99
MOTA	3341	OH2 TIP C		41.791	22.878	0.132	1.00 56.14
MOTA	3342	OH2 TIP C		7.088	25.685	41.540	1.00 47.43
		OH2 TIP C	223		4.785	13.582	1.00 47.96
ATOM	3343	002 717 0	227	40.690		15.174	1.00 48.76
MOTA	3344	OH2 TIP C	44	±0.030	4.360	10.1.	

MOTA	3345	OH2 TIP	С	225	10.029	32.425	18.562	1.00 36.30
	3346			226	22.346	37.737	48.941	1.00 34.15
MOTA								
MOTA	3347.			227	16.274	17.012	19.693	1.00 27.63
MOTA	3348	OH2 TIP	С	228	35.332	13.692	20.375	1.00 37.59
ATOM	3349			229	41.228	36.673	22.908	1.00 51.58
					17.416	42.030	50.226	1.00 47.63
MOTA	3350			230				
MOTA	3351	OH2 TIP	С	231	18.428	39.213	52.835	1.00 40.43
ATOM	3352	OH2 TIP	C	232	42.243	43.386	25.548	1.00 48.60
ATOM	3353			233	14.081	18.701	0.364	1.00 32.87
				234	41.421	41.332	28.531	1.00 54.67
ATOM	3354							
MOTA	3355			235	42.772	36.396	11.892	1.00 41.24
ATOM	3356	OH2 TIP	С	236	13.068	13.733	28.653	1.00 42.66
ATOM.	3357 ·	OH2 TIP	С	237	10.850	26.738	7.811	1.00 40.46
ATOM	3358		Ċ	238	16.253	20.926	45.776	1.00 44.60
					32.681	31.139	43.220	1.00 42.20
MOTA	3359			239				
ATOM	3360			240	56.267	22.254	9.280	1.00 52.44
ATOM	3361	OH2 TIP	C	241	12.553	25.304	9.942	1.00 38.77
MOTA	3362	OH2 TIP	C	242	50.727	9.516	16.775	1.00 33.38
ATOM	3363			243	31.871	41.347	0.512	1.00 47.78
				244	10.008	45.092	37.807	1.00 39.52
ATOM	3364							
MOTA	3365			245	14.551	39.030	6.708	1.00 44.26
MOTA	3366	OH2 TIP	С	246	26.955	18.903	-5.135	1.00 42.54
MOTA	3367	OH2 TIP	C	247	39.916	22.478	18.854	1.00 33.22
ATOM	3368		Ċ	248	40.431	40.824	22.426	1.00 35.58
		_		249	52.081	23.408	10.759	1.00 42.53
ATOM	3369							
ATOM	3370			250	12.078	16.710	24.149	1.00 32.37
MOTA	3371	OH2 TIP	С	251	54.111	15.908	8.256	1.00 44.58
MOTA	3372	OH2 TIP	C	252	33.950	12.827	-1.753	1.00 27.02
ATOM	3373			253	-0.775	26.703	40.353	1.00 43.64
				254	1.937	33.711	40.561	1.00 42.67
ATOM	3374							
ATOM	3375			255	8.008	24.066	18.824	1.00 51.45
MOTA	3376	OH2 TIP	С	256	11.765	27.465	3.635	1.00 47.34
MOTA	3377	OH2 TIP	C	257	27.863	43.878	9.233	1.00 32.44
ATOM	3378	OH2 TIP	C	258	18.655	30.114	4.303	1.00 33.13
	3379			259	21.592	19.085	-3.960	1.00 39.86
MOTA							25.906	1.00 26.34
ATOM	3380	OH2 TIP		260	41.876	24.067		
MOTA	3381			261	46.651	10.240	2.171	1.00 44.38
MOTA	3382	OH2 TIP	C	262	32.536	15.827	32.477	1.00 43.28
ATOM	3383	OH2 TIP	C	263	12.479	39.205	50.359	1.00 47.33
ATOM	3384			264	0.850	27.980	38.316	1.00 43.45
				265	49.605	7.356	18.061	1.00 66.01
MOTA	3385							
MOTA	3386	OH2 TIP			30.177	40.365	-3.235	1.00 44.45
ATOM	3387	OH2 TIP	C	267	39.818	12.364	0.512	1.00 48.84
ATOM	3388	OH2 TIP	C	268	38.149	44.716	27.884	1.00 51.18
ATOM	3389	OH2 TIP	C	269	37.156	37.062	30.528	1.00 35.17
ATOM	3390	OH2 TIP				7.097	12.435	1.00 51.69
							12.471	1.00 47.45
MOTA	3391	OH2 TIP			54.351	12.626		
MOTA	3392	OH2 TIP			50.835		13.092	1.00 55.05
MOTA	3393	OH2 TIP	С	273	12.159	35.313	52.133	1.00 52.38
ATOM	3394	OH2 TIP			21.002	44.489	13.037	1.00 39.70
ATOM	3395	OH2 TIP			37.936		34.221	1.00 48.56
								1.00 43.24
MOTA	3396	OH2 TIP			45.844	30.935	31.365	
MOTA	3397	OH2 TIP			38.831	48.015	15.554	1.00 49.83
MOTA	3398	OH2 TIP	C	278	5.630	28.150	44.576	1.00 48.10
ATOM	3399	OH2 TIP			8.600	24.000	45.727	1.00 49.27
ATOM	3400	OH2 TIP			54.276		7.807	1.00 36.02
					3.544		46.365	1.00 43.63
ATOM	3401	OH2 TIP						
ATOM	3402	OH2 TIP			24.214			1.00 48.04
MOTA	3403	OH2 TIP			7.099		19.549	1.00 54.97
MOTA	3404	OH2 TIP	С	284	36.469		41.355	1.00 52.17
ATOM	3405	OH2 TIP			34.660		23.756	1.00 45.46
ATOM	3406	OH2 TIP			28.516	42.981	5.402	1.00 53.58
MION	2400	OHZ TIP	·	200	20.010			

MOTA	3407	OH2	TIP				35.579	4.929		1.00	
MOTA	3408	OH2	TIP	С	288		22.974	49.682		1.00	
MOTA	3409	OH2	TIP	С	289		3.725	31.464	46.354		46.43
ATOM	3410	OH2	TIP	С	290		27.340	39.594	-2.191	1.00	56.89
ATOM	3411	OH2	TIP		291		33.413	34.856	32.335	_	31.78
ATOM	3412	OH2	TIP		292		43.340	7.715	8.063	1.00	43.53
ATOM	3413	OH2	TIP		293		28.243	21.392	-4.937	1.00	38.33
ATOM	3414	OH2	TIP		294		49.389	26.590		1.00	45.66
			TIP				28.948	15.824			52.48
ATOM	3415	OH2	TIP		295 296		27.347	13.383			48.27
ATOM	3416	OH2					38.485	26.090			48.92
MOTA	3417	OH2	TIP					20.265			50.10
ATOM	3418	OH2	TIP				12.120	36.306			50.38
ATOM	3419	OH2	TIP				36.480				38.37
MOTA	3420	OH2	TIP	-	300		31.471	16.463			33.49
ATOM	3421	OH2	TIP				42.889	5.274			39.09
MOTA	3422	OH2	TIP	_	302		23.548	44.173			52.67
ATOM	3423	OH2	TIP				13.465	43.978			52.07
MOTA	3424	OH2	TIP		304		25.133	43.053			
MOTA	3425	OH2	TIP				33.587	24.652			49.48
ATOM	3426	OH2	TIP				39.063	28.353			47.89
ATOM	3427	OH2	TIP	С	307		49.357	35.834			49.22
MOTA	3428	OH2	TIP	С	308		27.159	46.386			49.50
MOTA	3429	OH2	TIP	С	309		9.510	21.769			47.95
ATOM	3430	OH2	TIP	С	310		34.885	32.959			51.26
MOTA	3431	OH2	TIP	С	311		30.980	6.002			56.02
ATOM	3432	OH2	TIP	С	312		43.802	34.511			41.89
ATOM	3433	OH2	TIP		313	•	36.834	4.382	5.254		39.04
ATOM	3434	OH2	TIP		314		12.453	30.429	47.461	1.00	47.60
ATOM	3435	OH2	TIP		315		39.685	40.144	30.944	1.00	54.68
ATOM	3436	OH2	TIP				45.982	20.840	31.078	1.00	47.99
ATOM	3437	OH2	TIP				32.815	36.023	42.050	1,00	45.07
ATOM	3438	OH2	TIP		318		17.877	37.802	-3.699	1.00	56.30
	3439	OH2	TIP		319		53.681	9.633		1.00	55.34
ATOM	3440	OH2	TIP				21.577	43.070		1.00	49.54
ATOM	3441	OH2	TIP				6.139	45.122		1.00	44.40
MOTA	3442	OH2			322		34.695	13.561			45.99
MOTA	3443	OH2	TIP	_	323		17.990	33.946			56.88
MOTA	3444	OH2	TIP		324		25.587	50.416			52.75
MOTA		OH2	TIP				27.744	42.608			44.66
MOTA	3445	OH2			326		48.357	32.815			57.98
MOTA	3446	OH2			327		61.047	18.004			51.30
MOTA	3447	OH2					17.327	11.069		1.00	48.28
MOTA	3448						59.624	17.562			44.37
MOTA	3449	OH2	TIP				40.644	39.227			37.57
MOTA	3450	OH2					12.920	31.214			51.07
MOTA	3451						37.639	0.847			49.44
ATOM	3452		TIP				34.243	38.790			54.21
ATOM	3453	OH2					24.216	47.874		_	50.90
MOTA	3454	OH2					15.324	34.79			45.25
MOTA	3455	OH2			335		18.474				34.12
MOTA	3456	OH2							_	_	49.89
MOTA	3457	OH2					40.048	8.873			29.86
MOTA	3458	OH2					32.472	13.33			49.76
MOTA	3459	OH2					57.778	14.16			56.48
MOTA	3460	OH2					46.651	35.47			5725
MOTA	3461		TIP				15.427	13.23			65.27
ATOM	3462	OH2					40.349	38.97			59.60
ATOM	3463	OH2					8.685	28.94			37.18
MOTA	3464	OH2			344		11.958	41.58			42.95
MOTA	3465		TIP				9.054	20.49			42.93
MOTA	3466	OH2			346		20.086	20.08			42.03
ATOM	3467	OH2			347		40.370				
MOTA	3468	OH2	TIP	C	348		41.948	4.32	7 12.147	1.00	50.59

MOTA MOTA MOTA	3469 3470 3471	OH2	TIP C TIP C	350	23.518 19.169 32.946	45.701 37.474 39.184	40.287 4.786 41.062	1.00 39.79 1.00 44.67 1.00 57.56
ATOM ATOM	3472 3473		TIP C		37.578 15.391	47.817 43.820	18.421 7.645	1.00 51.80 1.00 58.15
ATOM ATOM	3474 3475	OH2	TIP C	355	38.205 43.224	17.257	33.401 14.606	1.00 55.84 1.00 41.12
ATOM ATOM	3476 3477	OH2	TIP C	357	18.704 46.033	51.623	28.487	1.00 61.11
ATOM ATOM ATOM	3478 3479 3480	OH2	TIP C TIP C	359	51.950 46.825 17.624	27.722 2.427 50.111	14.408 15.714 20.315	1.00 45.00 1.00 52.68 1.00 39.65
ATOM ATOM	3481 3482	0	HOH C	361	27.534 28.946	15.877	26.687	1.00 20.00
END		-						

## INTERNATIONAL SEARCH REPORT

International application No.

PCT/US01/29387

		1 0 17 0 20 21 27 20 2	
A. CLA IPC(7)	SSIFICATION OF SUBJECT MATTER : G01N 33/483		
US CL	: 702/19		
	International Patent Classification (IPC) or to both	national classification and IPC	
	DS SEARCHED	11 \ '5'	
	ocumentation searched (classification system followed 702/17, 435, 424.	i by classification symbols)	
Documentati	ion searched other than minimum documentation to th	ne extent that such documents are include	d in the fields searched
	ata base consulted during the international search (na Continuation Sheet	me of data base and, where practicable, s	search terms used)
C. DOC	UMENTS CONSIDERED TO BE RELEVANT		
Category *	Citation of document, with indication, where a	ppropriate, of the relevant passages	Relevant to claim No.
Y	ROSSJOHN et al. Crystal structure of the N-termir Alzheimer amyloid precursor protein. Nature Structure, pages 327-331, see entire document and especial	tural Biology. April 1999, Vol 6. No.	1-2
Y	ZHANG Z. et al. Sequence-specific recognition of Alzheimer's amyloid precursor protein by the X11 1997, Vol 16. No. 20, pages 6141-6150, see entire document and especially page 6147.	the interanalization motif of the PTB domain. The EMBO Journal.	1-2
Y,P	MARCINKEVICIENE J. at al. Mechanism of Inhi Protein-cleaving Enzyme (BACE) by a Statine-base Chemistry. 29 June 2001, Vol 276, No. 26, pages	ed Peptide. The Journal of Biological	1
Y	HYNES et al. X-ray Crystal Structure of the Protes Amyloid beta-Protein Precursor. Biochemistry. 199 especially page 10019.	ase Inhibitor Domain of Alzheimer's 10, Vol 29, pages 10018-10022,	1-2
	<u> </u>		
Furthe	er documents are listed in the continuation of Box C.	See patent family annex.	
•	Special categories of cited documents:	"T" later document published after the inte date and not in conflict with the applic	
1	nd defining the general state of the art which is not considered to be sular relevance	principle or theory underlying the invention of particular relevance; the	
ł	application or patent published on or after the international filing date	considered novel or cannot be consider when the document is taken alone	red to involve an inventive step
establish specified		"Y" document of particular relevance; the considered to involve an inventive step combined with one or more other sunbeing obvious to a person skilled in the	when the document is a document, such combination
1	nt referring to an oral disclosure, use, exhibition or other means at published prior to the international filing date but later than the	"&" document member of the same patent	,
priority	date claimed		
1	actual completion of the international search	Date of mailing of the international sea	2002
	er 2001 (18.12.2001) nailing address of the ISA/US	Authorized officer	ex Im
Co	mmissioner of Patents and Trademarks	Lana Dridg	
W	x PCT ashington, D.C. 20231	Tolon No. (702) 208 0106	LITSKY PhD.
Facsimile N	lo. (703)305-3230	Telephone No. (703)-308-0196	

Form PCT/ISA/210 (second sheet) (July 1998)

International application No.

PCT/US01/29387

# INTERNATIONAL SEARCH REPORT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	BAILEY et al. X-ray-crystallographic studies of complexes of pepstatin A and a statine-containing human renin inhibitor with endothiapepsin. Biochem. J.1993, Vol 289, pages 363-371, especialy pages 365-366.	1-2
Y	SCHEIDIG et al. Crystal structures of bovin chymotrypsin and trypsin complexed to the inhibitor domain of Alzheimer's amyloid beta-protein precursor (APPI) and basic pancreatic trypsin inhibitor (BPTI): Engineering of inhibitors with altered specificities. The Protein Society. September 1997, Vol 6, pages 1806-1824, see entire document and especially page 1820.	1-2
A	KOHNO et al. Thre-Dimentional Structure of the Amyloid beta Peptide (25-35) in Membrane-Mimicking Environment. Biochemistry. 1996, Vol 35, pages 16094-16104, see entire document.	1-2
A	VASSAR et al. Beta-Secretase Cleavage of Azheimer's Amyloid Precursor Protein by the Transmembrane Aspartic Protease BACE. Science. 22 October 1999, Vol 286, pages 735-741, see entire document.	1 <b>-2</b>
<b>A</b>	HONG, L. et al. Structure of the Protease Domain of Memapsin 2(beta-Secretase) Complexed with Inhibitor. Science. 24 May 2000, Vol 290, No. 5489, pages 150-159, see entire document	1-2
A	SAUDER, M. et al. Modeling of substrate specifity of the Alzheimer's desease amyloid precursor protein beta-secretase. J. Mol. Biol. 2000, Vol 300, No. 2, pages 241-248, see entire document.	1-2
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## INTERNATIONAL SEARCH REPORT

International application No.

PCT/US01/29387

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)	
This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:	
1. Claim Nos.: because they relate to subject matter not required to be searched by this Authority, namely:	
Claim Nos.: because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:	
3. Claim Nos.:  because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).	
Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)	
This International Searching Authority found multiple inventions in this international application, as follows: Please See Continuation Sheet	
1. As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.	
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.	
3. As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.: 1 and 2	
4. No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:	
Remark on Protest	
No protest accompanied the payment of additional search fees.	
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INTERNATIONAL SEARCH REPUB	TERNATIONAL SEAR	CH REPOR	T
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International application No.

PCT/US01/29387

### BOX II. OBSERVATIONS WHERE UNITY OF INVENTION IS LACKING

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Invention I and II are directed to different chemical and physical types regarding the critical limitations therein. For Group I, the critical feature is a crystallization of complex whereas for Group II the critical feature is the obtaining or synthesizing the agent. This application contains the following inventions or groups of inventions which are not so linked as to form a single general inventive concept under PCT Rule 13.1. In order for all inventions to be searched, the appropriate additional examination fees must be paid.

Group I, claims 1-2, drawn to crystallized complex.

Group II, claims 24 and 27 drawn to method further comprising one of the steps: obtaining and synthesizing the agen. Claims 3-23, 25,26,28-30 are directed solely to information and are therefore excluded from search.

The International Searching Authority considers that the international application does not comply with the requirements of unity of invention (Rules 13.1, 13.2 and 13.3) for reasons indicated below:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Invention I and II are directed to different chemical and physical types regarding the critical limitations therein. For Group I, the critical feature is a crystallization of complex whereas for Group II the critical feature is the obtaining or synthesizing the agent.

### Continuation of B. FIELDS SEARCHED Item 3:

WEST, STN, Non-patent-literature covering search terms: Cleaving Enzyme(BACE), crystallization, beta-Amyloid Precursor protein, 3-d structure of APP, Statine-based peptides.

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